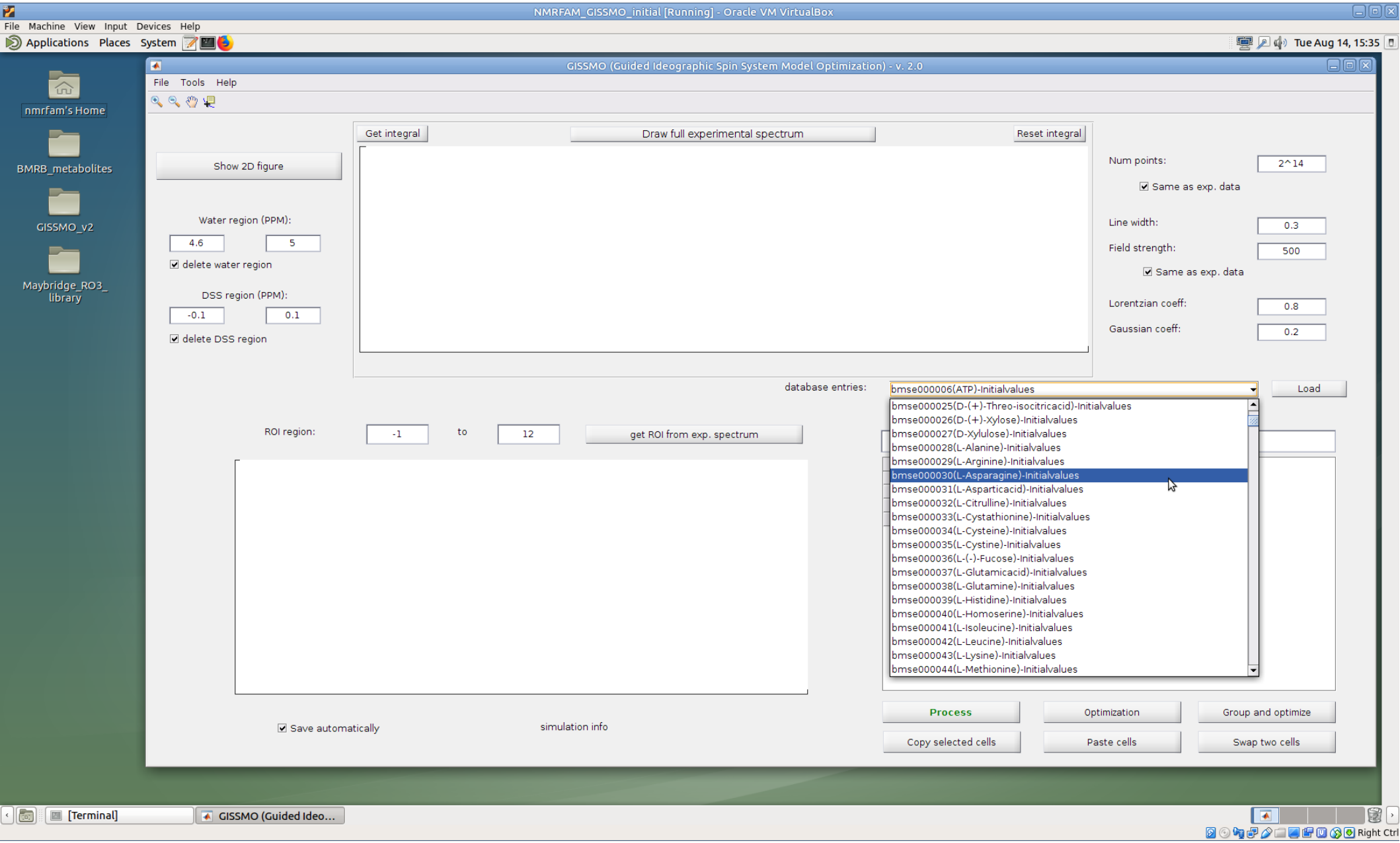
NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
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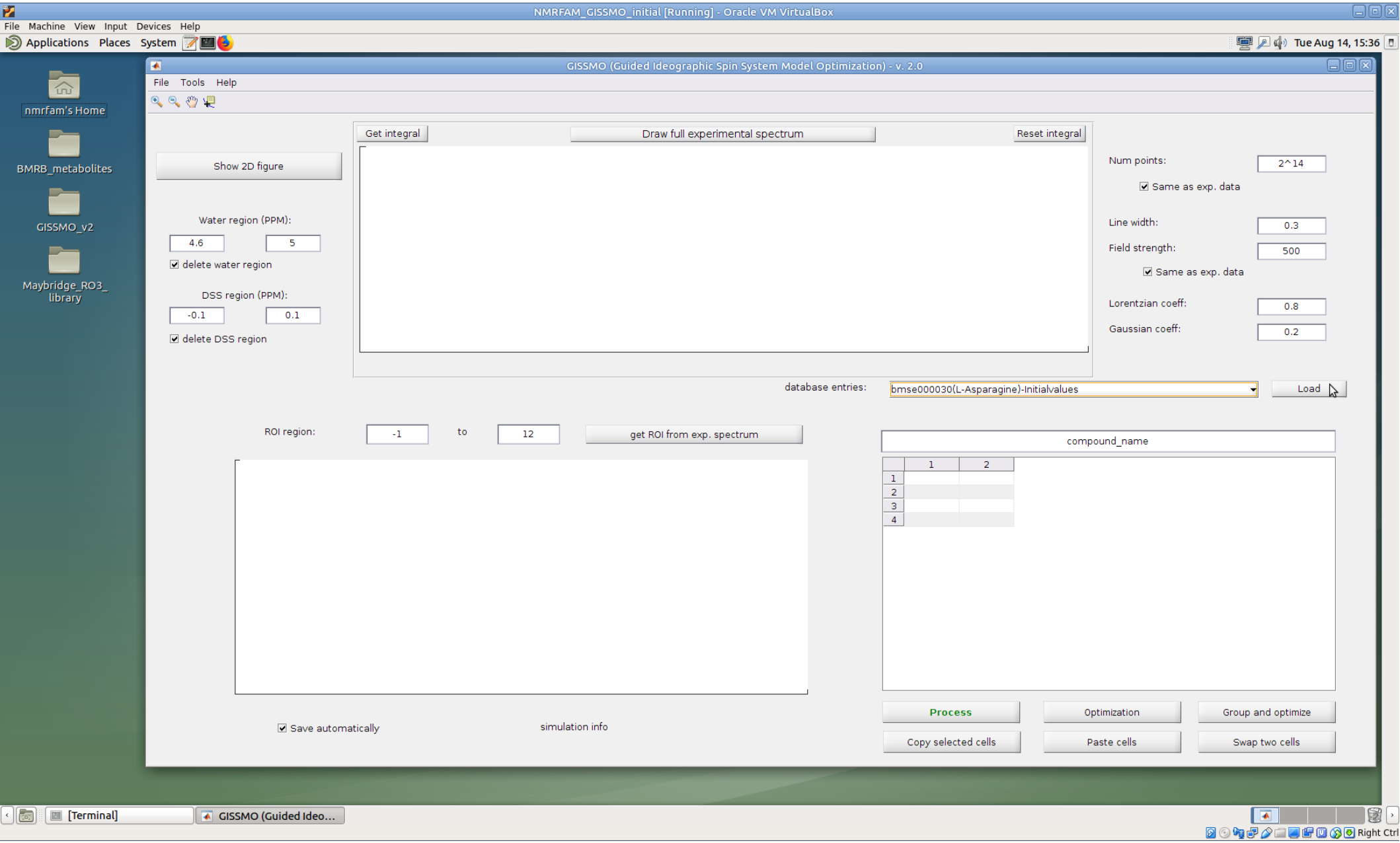
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Num points:
2^14
Same as exp. data
Water region (PPM):
4.6
5
delete water region
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:
bmse000006(ATP)-Initialvalues
Load
bmse000025(D-(+)-Threo-isocitricacid)-Initialvalues
bmse000026(D-(+)-Xylose)-Initialvalues
bmse000027(D-Xylulose)-Initialvalues
bmse000028(L-Alanine)-Initialvalues
bmse000029(L-Arginine)-Initialvalues
bmse000030(L-Asparagine)-Initialvalues
bmse000031(L-Asparticacid)-Initialvalues
bmse000032(L-Citrulline)-Initialvalues
bmse000033(L-Cystathionine)-Initialvalues
bmse000034(L-Cysteine)-Initialvalues
bmse000035(L-Cystine)-Initialvalues
bmse000036(L-(-)-Fucose)-Initialvalues
bmse000037(L-Glutamicacid)-Initialvalues
bmse000038(L-Glutamine)-Initialvalues
bmse000039(L-Histidine)-Initialvalues
bmse000040(L-Homoserine)-Initialvalues
bmse000041(L-Isoleucine)-Initialvalues
bmse000042(L-Leucine)-Initialvalues
bmse000043(L-Lysine)-Initialvalues
bmse000044(L-Methionine)-Initialvalues
ROI region:
-1
to
12
get ROI from exp. spectrum
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
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BMRB_metabolites
GISSMO_v2
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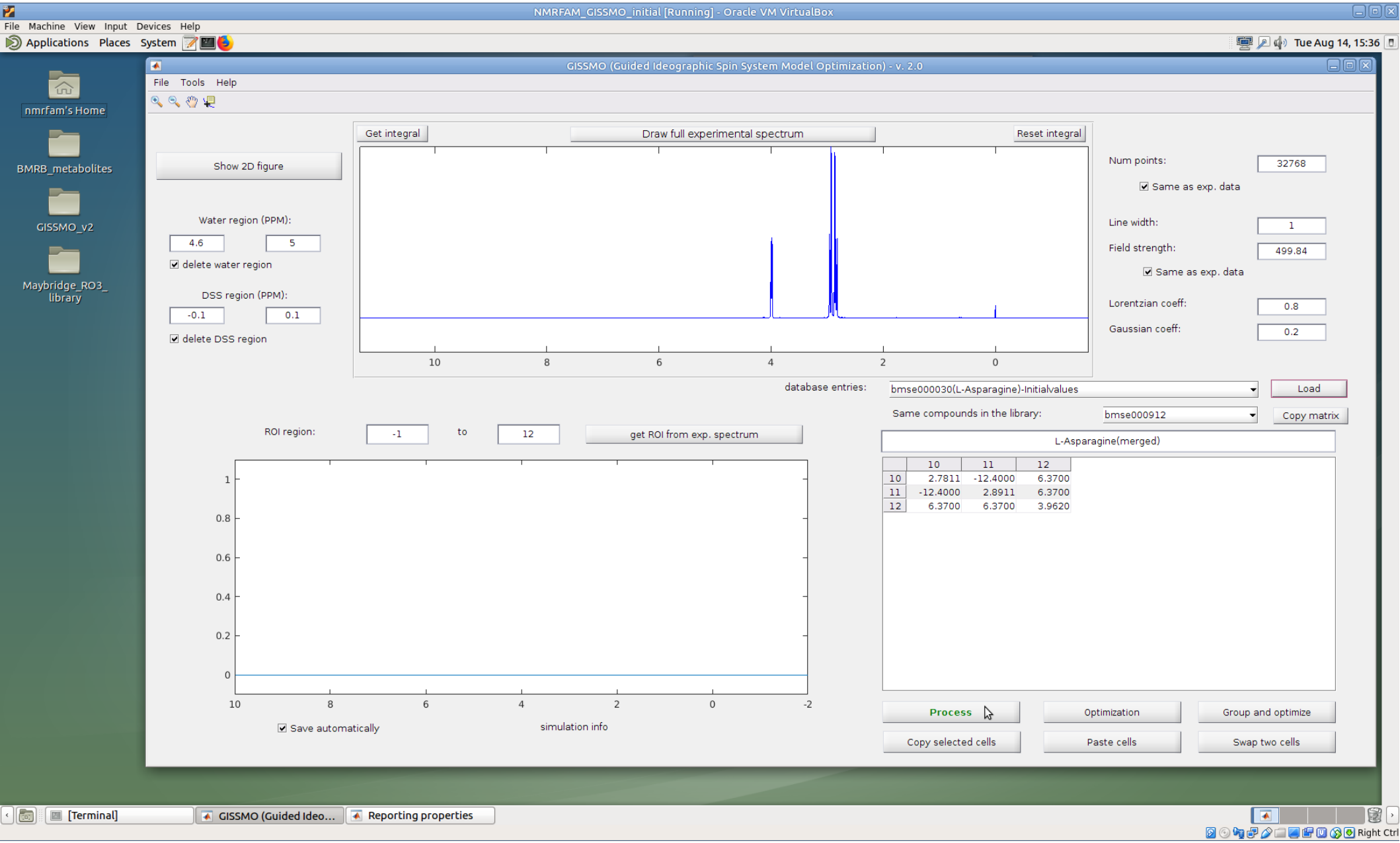
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Num points:
2^14
Same as exp. data
Water region (PPM):
4.6
5
delete water region
Line width:
0.3
Field strength:
500
Same as exp. data
DSS region (PPM):
-0.1
0.1
delete DSS region
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000030(L-Asparagine)-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 Ideo...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
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nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
10 8 6 4 2 0
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:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.7811 -12.4000 6.3700
11 -12.4000 2.8911 6.3700
12 6.3700 6.3700 3.9620
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 Ideo...
Reporting properties
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

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BMRB_metabolites

GISSMO_v2

Maybridge_RO3_ library

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset integral

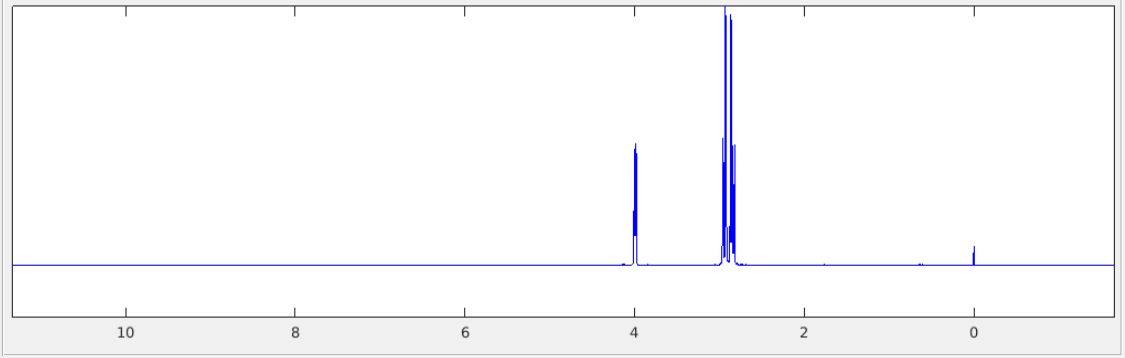
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

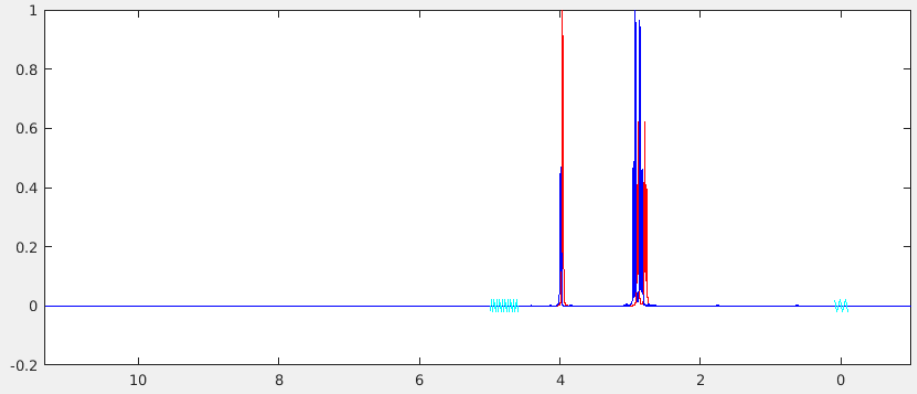
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

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



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

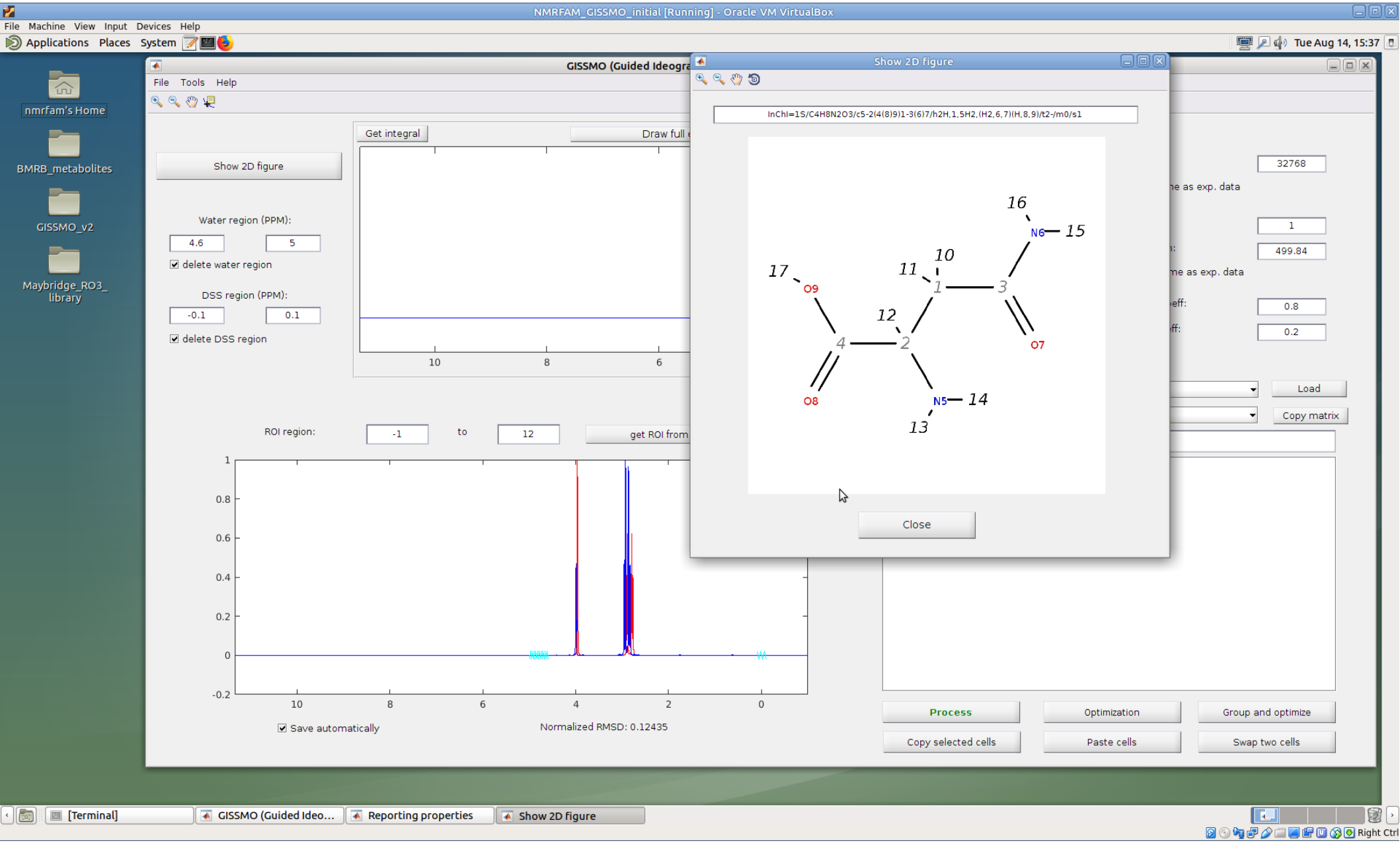
	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] GISSMO (Guided Ideo... Reporting properties

Right Ctrl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BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideogra
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full
ROI region:
-1
to
12
get ROI from
Save automatically
Normalized RMSD: 0.12435
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
O9
O8
O7
N6
N5
Close
32768
499.84
0.8
0.2
Load
Copy matrix
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

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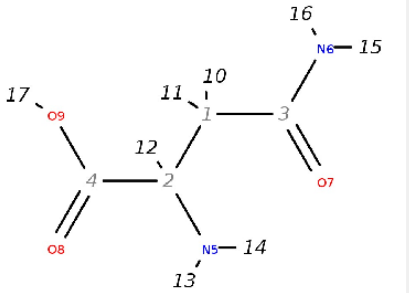
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

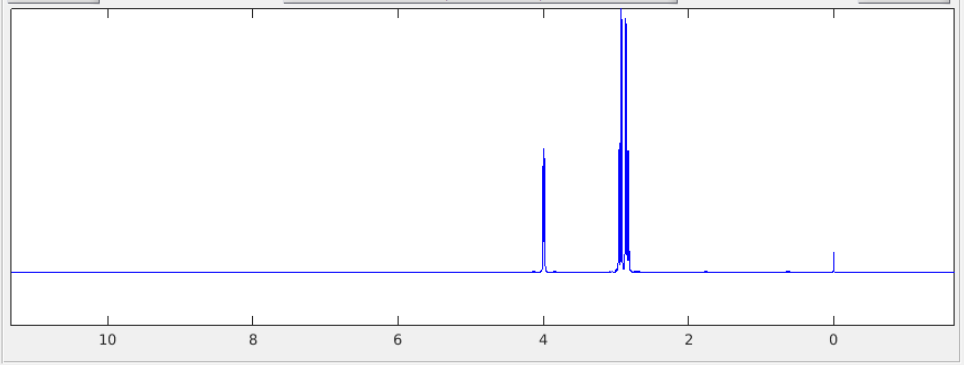
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

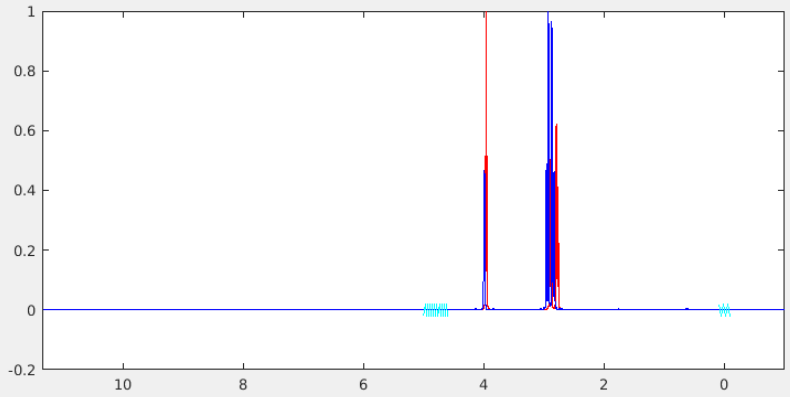
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

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



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

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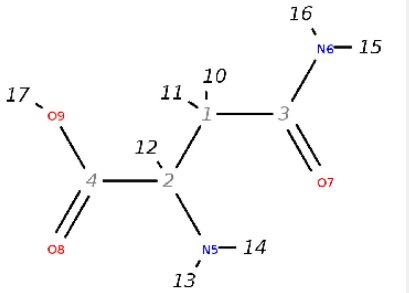
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

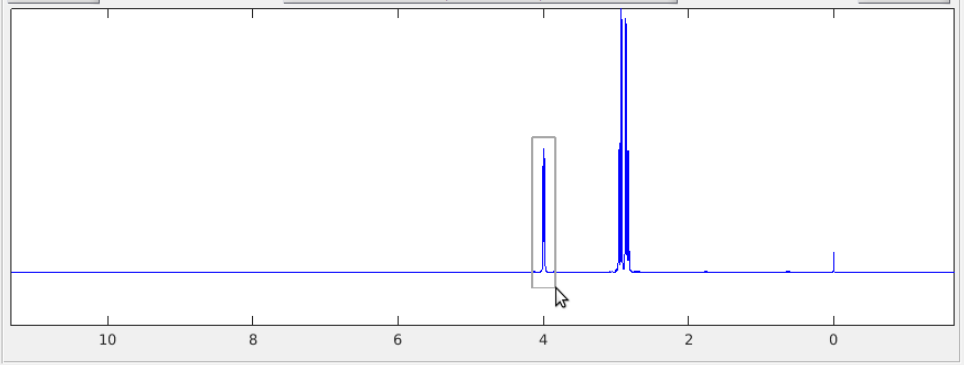


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

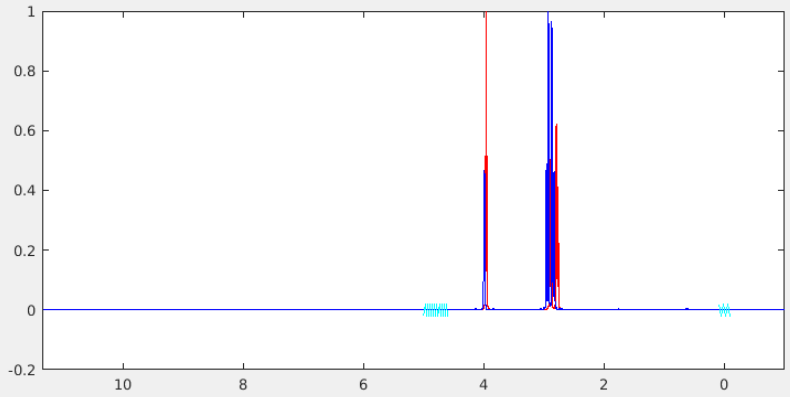
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

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



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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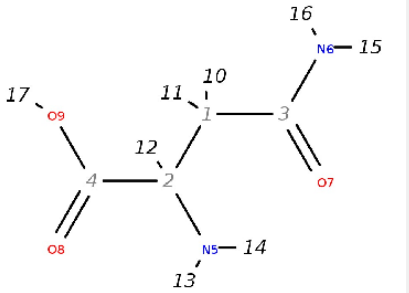
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

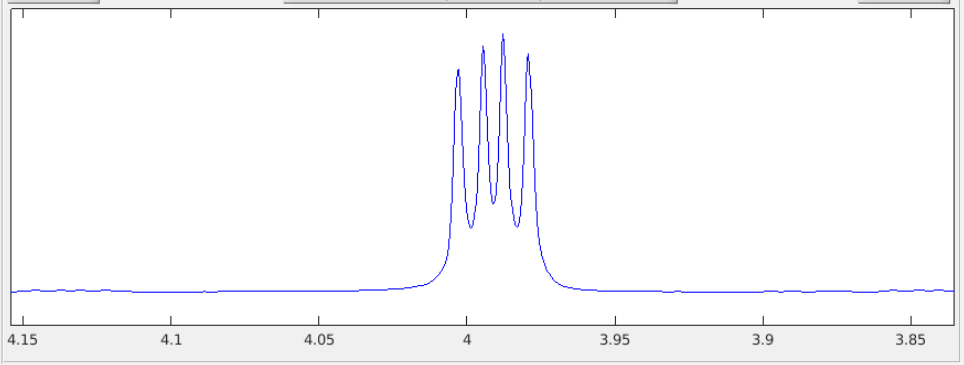
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

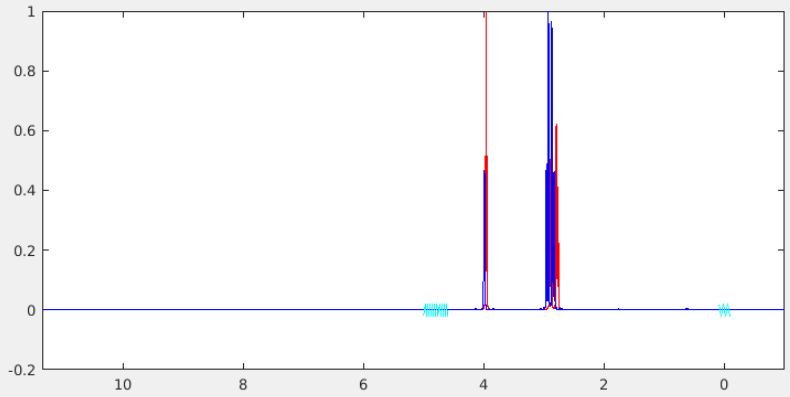
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

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



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

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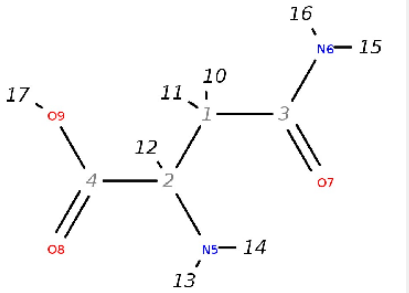
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

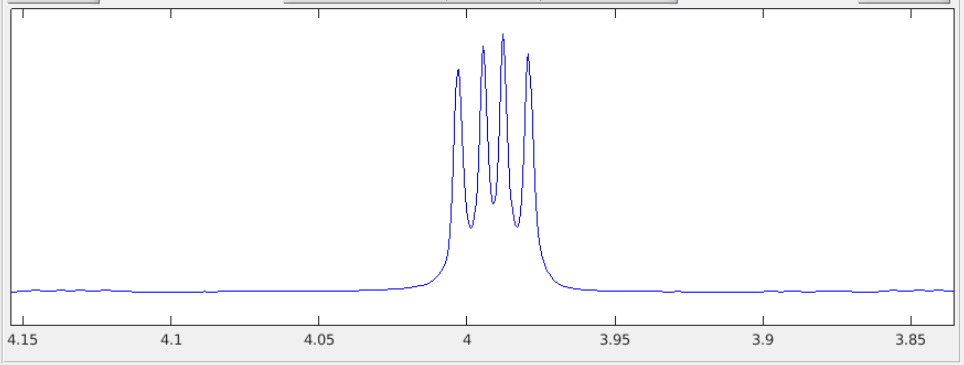
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

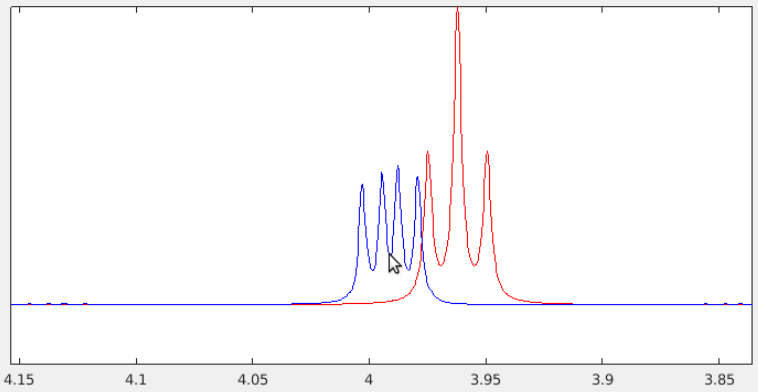
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

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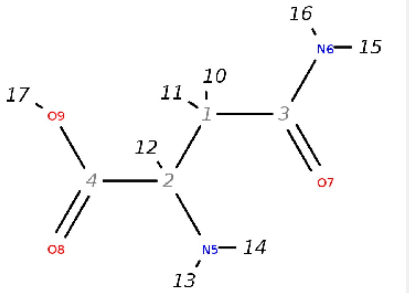
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

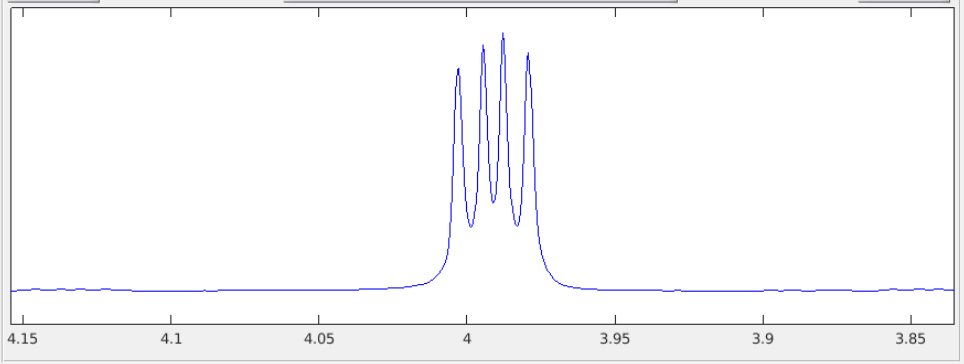
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

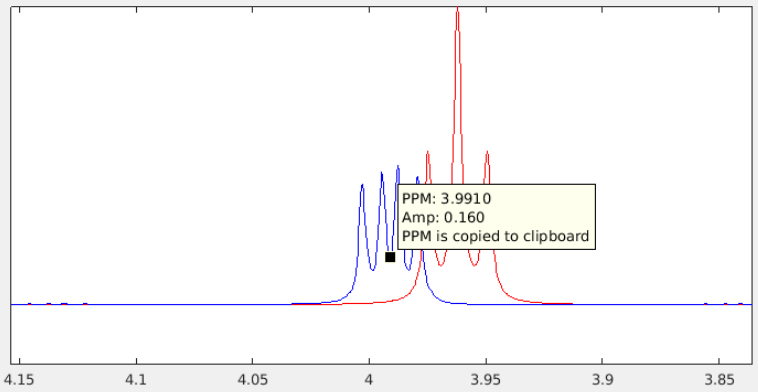
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9620

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

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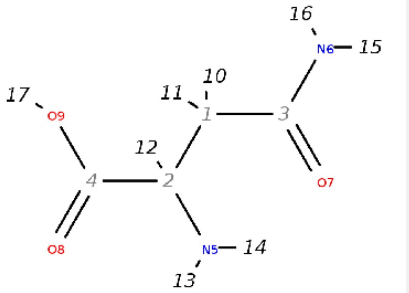
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

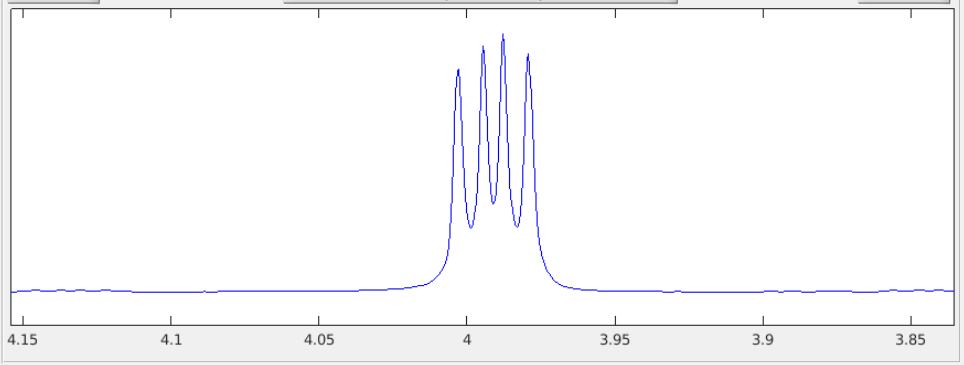


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

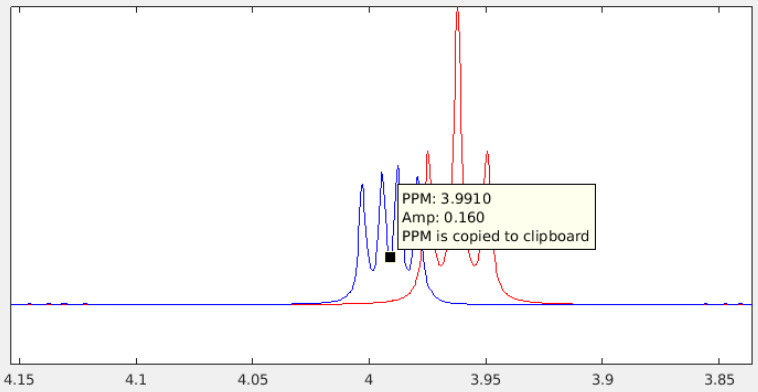
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 3.836 to 4.154 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12435

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

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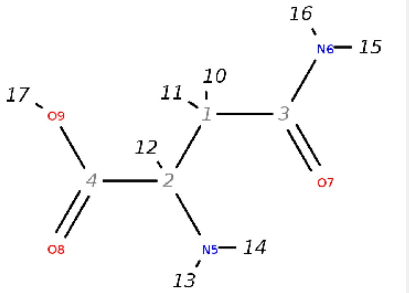
Tue Aug 14, 15:40

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

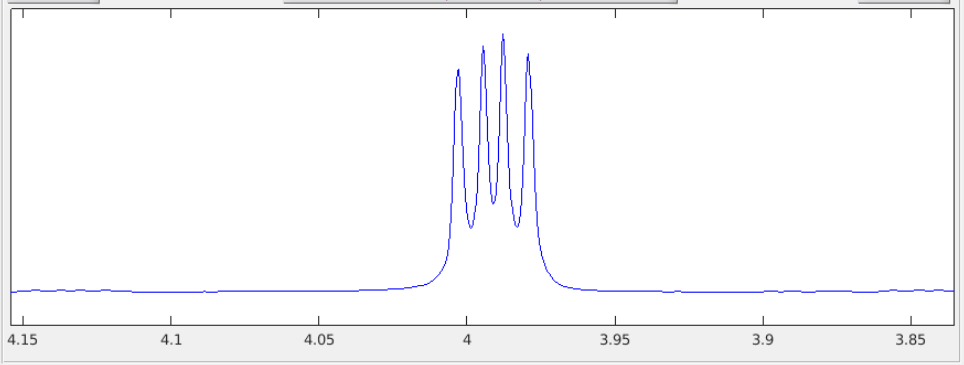
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

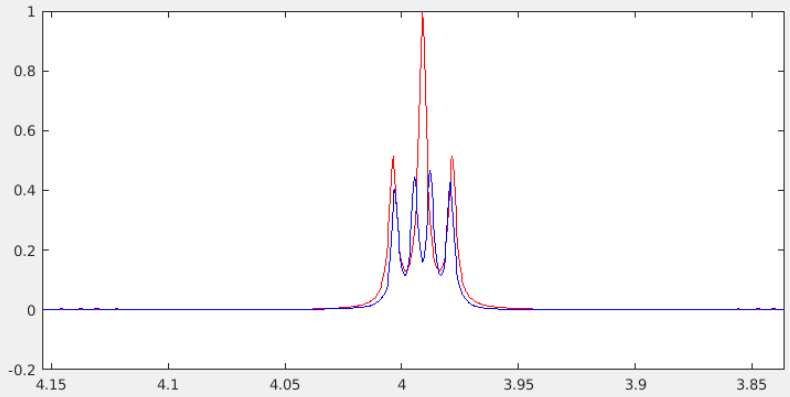
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10812

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3700
11	-12.4000	2.8911	6.3700
12	6.3700	6.3700	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

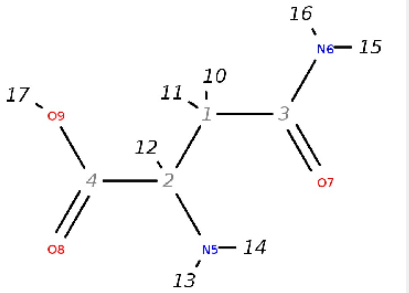
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:40

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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

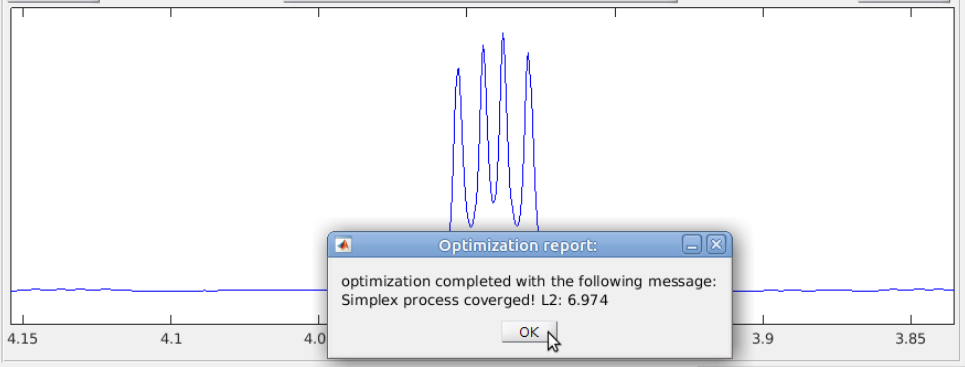
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 6.974

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

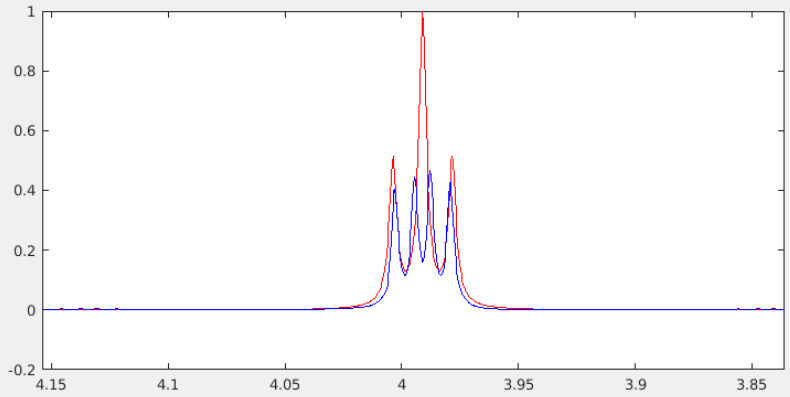
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10812

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3315
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

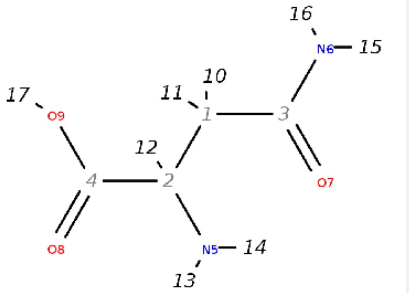
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:40

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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

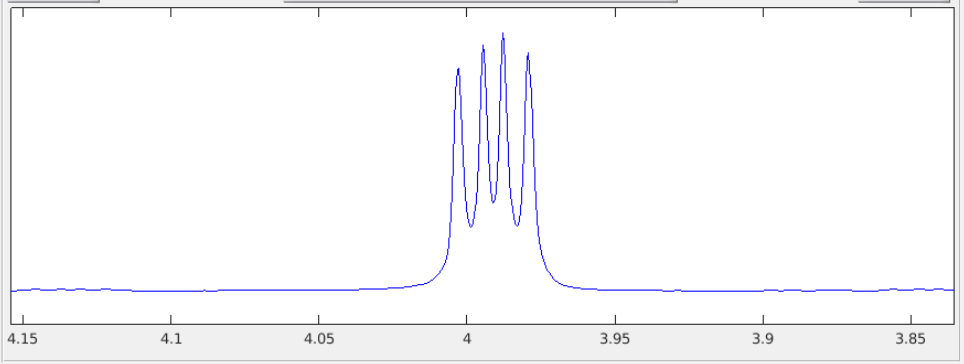
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

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Gaussian coeff: 0.2

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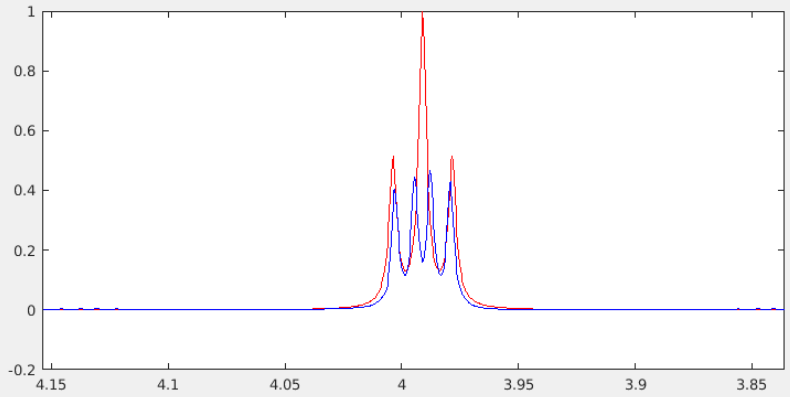
ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10812

L-Asparagine(merged)

	10	11	12
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11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

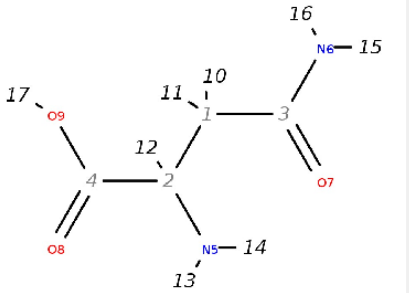
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:41

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

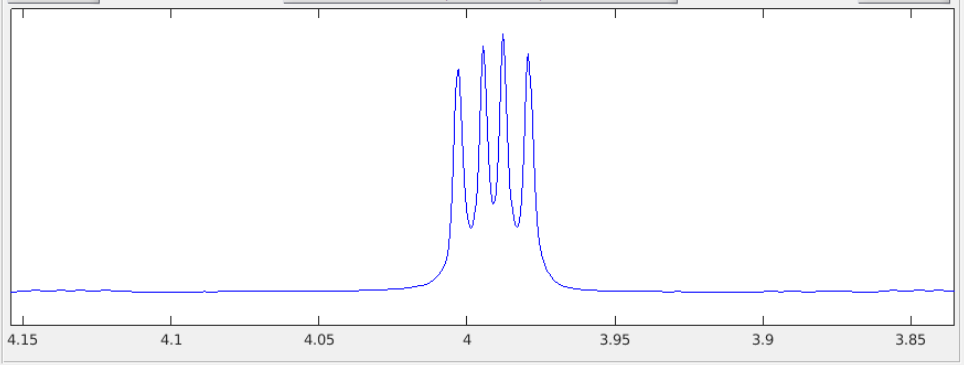
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

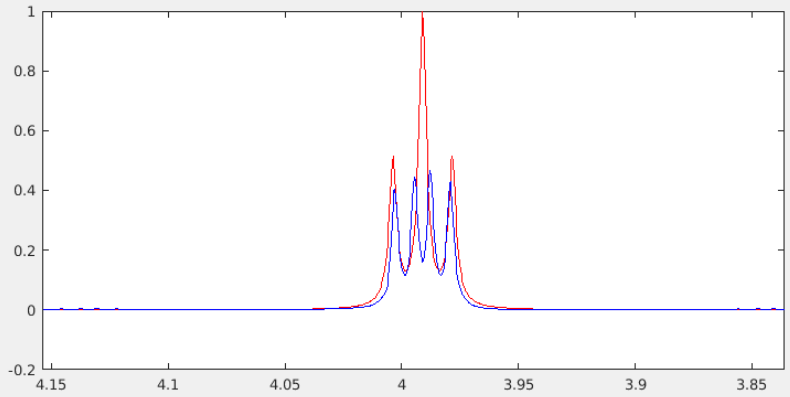
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

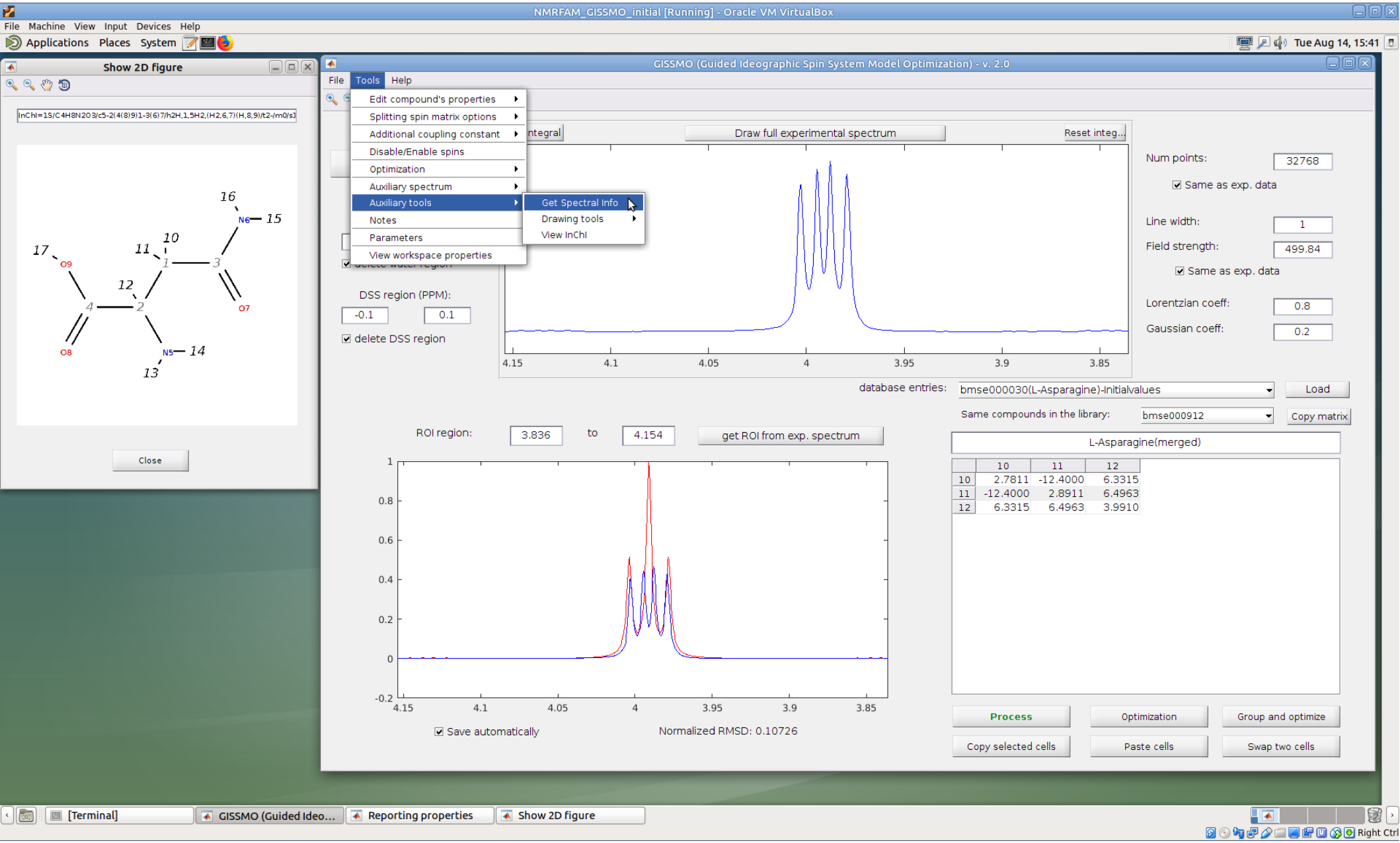
	10	11	12
10	2.7811	-12.4000	6.3315
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:41
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
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
Get Spectral Info
Drawing tools
View InChI
Draw full experimental spectrum
Reset integ...
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:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
3.836
to
4.154
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.7811 -12.4000 6.3315
11 -12.4000 2.8911 6.4963
12 6.3315 6.4963 3.9910
Save automatically
Normalized RMSD: 0.10726
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

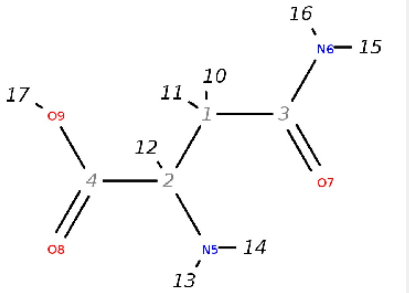
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:42

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

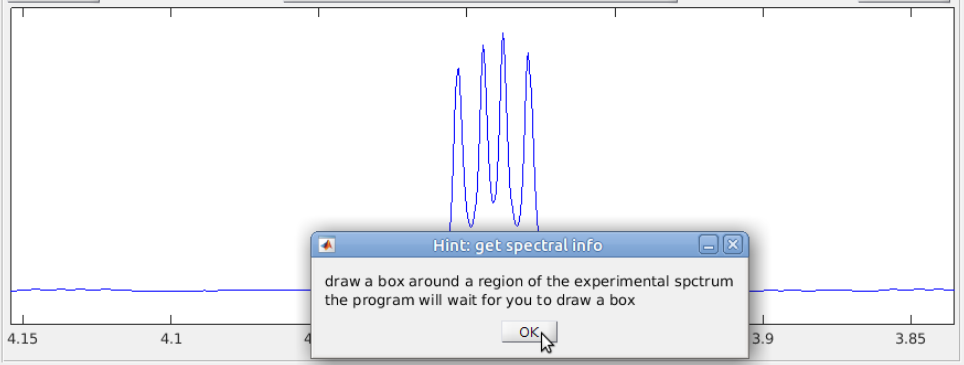


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Hint: get spectral info

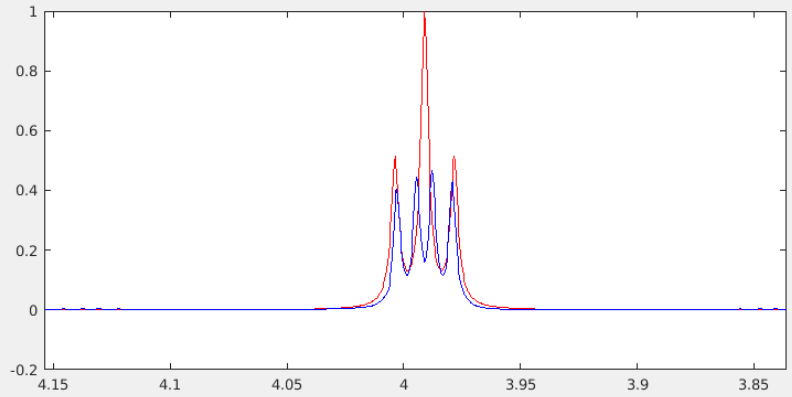
draw a box around a region of the experimental spctrum
the program will wait for you to draw a box

OK

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3315
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Hint: get spectral info

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

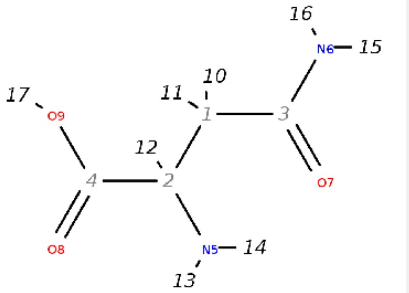
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:42

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

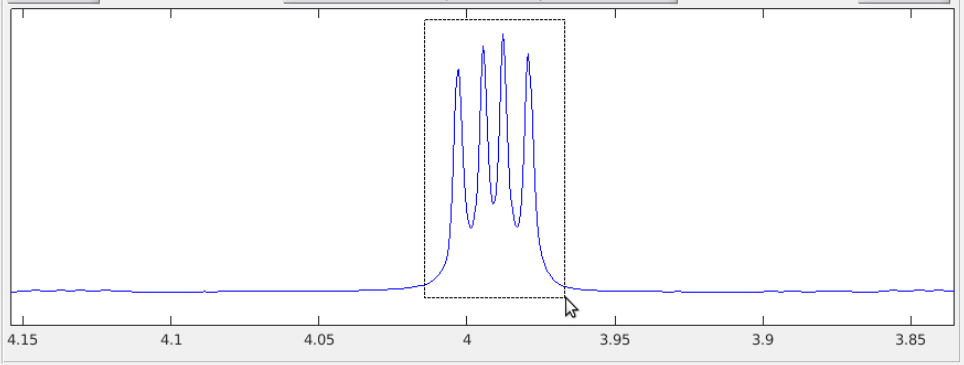
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

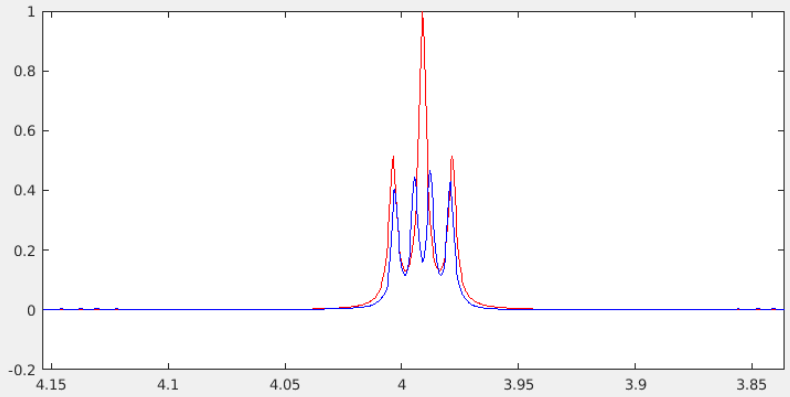
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	6.3315
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

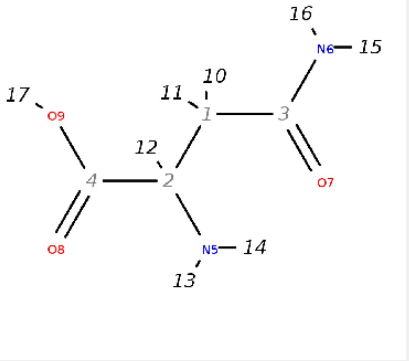
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:42

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

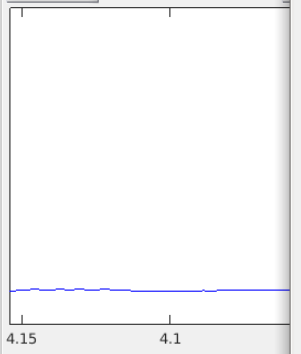
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

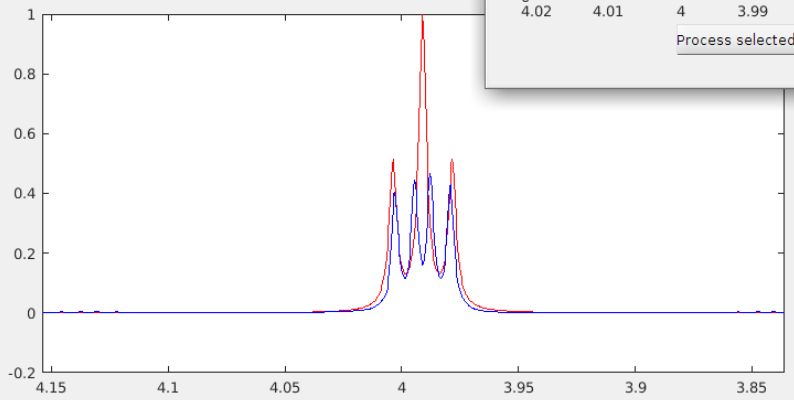
delete DSS region

Get integral



Reset integ...

ROI region: 3.836 to 4.154



Save automatically

Normalized RMSD: 0.10726

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

aragine)-Initialvalues Load

the library: bmse000912 Copy matrix

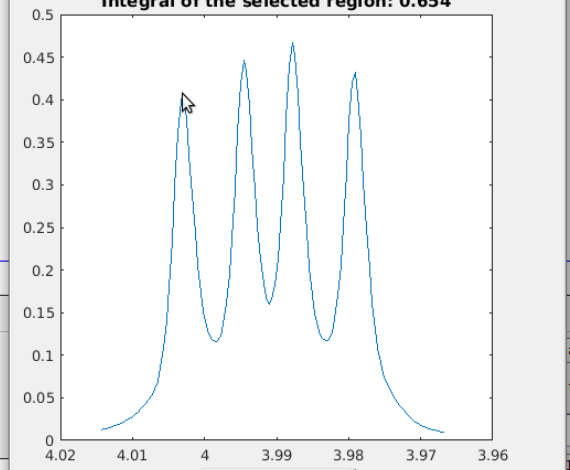
L-Asparagine(merged)

	12
4000	6.3315
8911	6.4963
4963	3.9910

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

Get info from experimental data

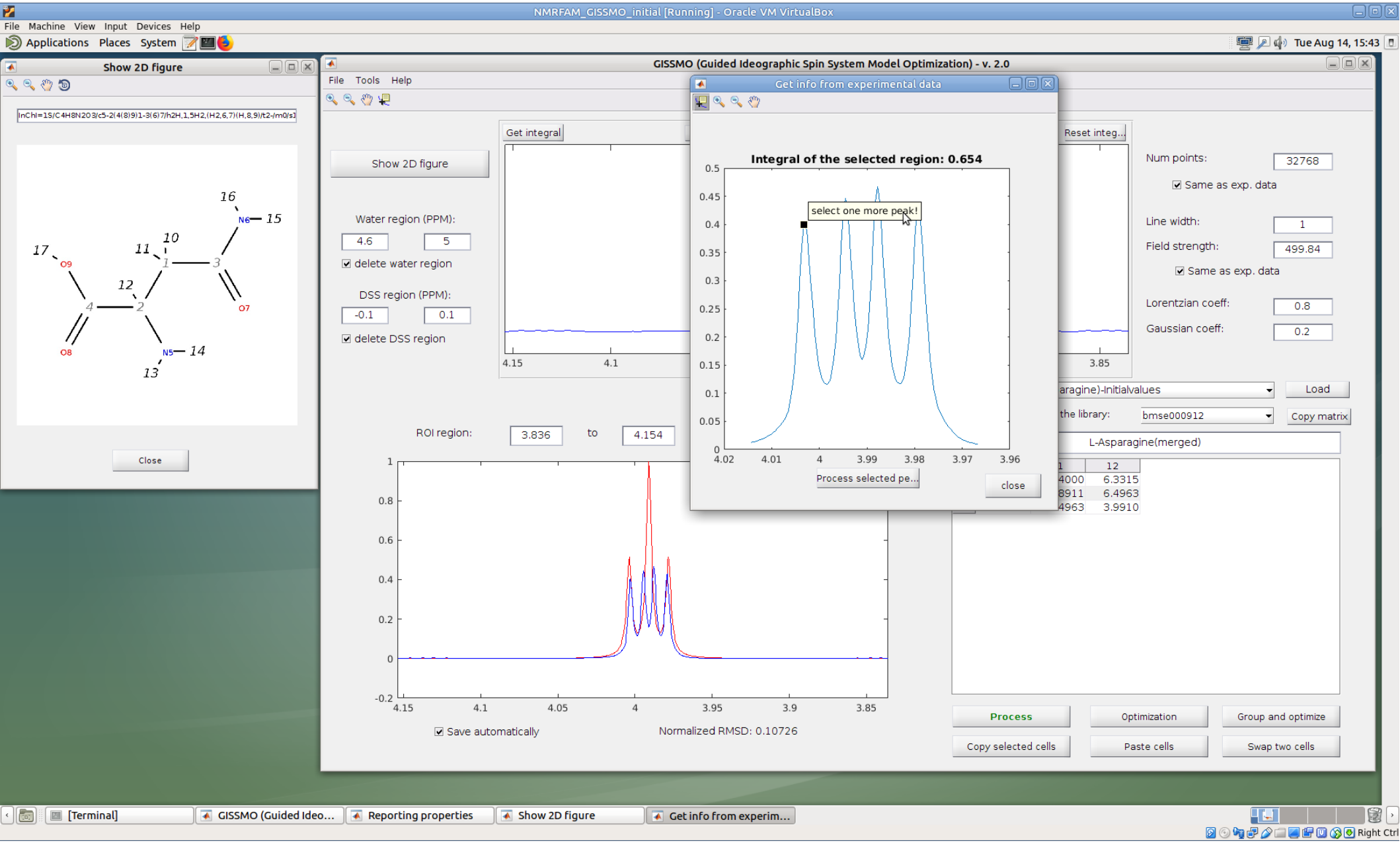


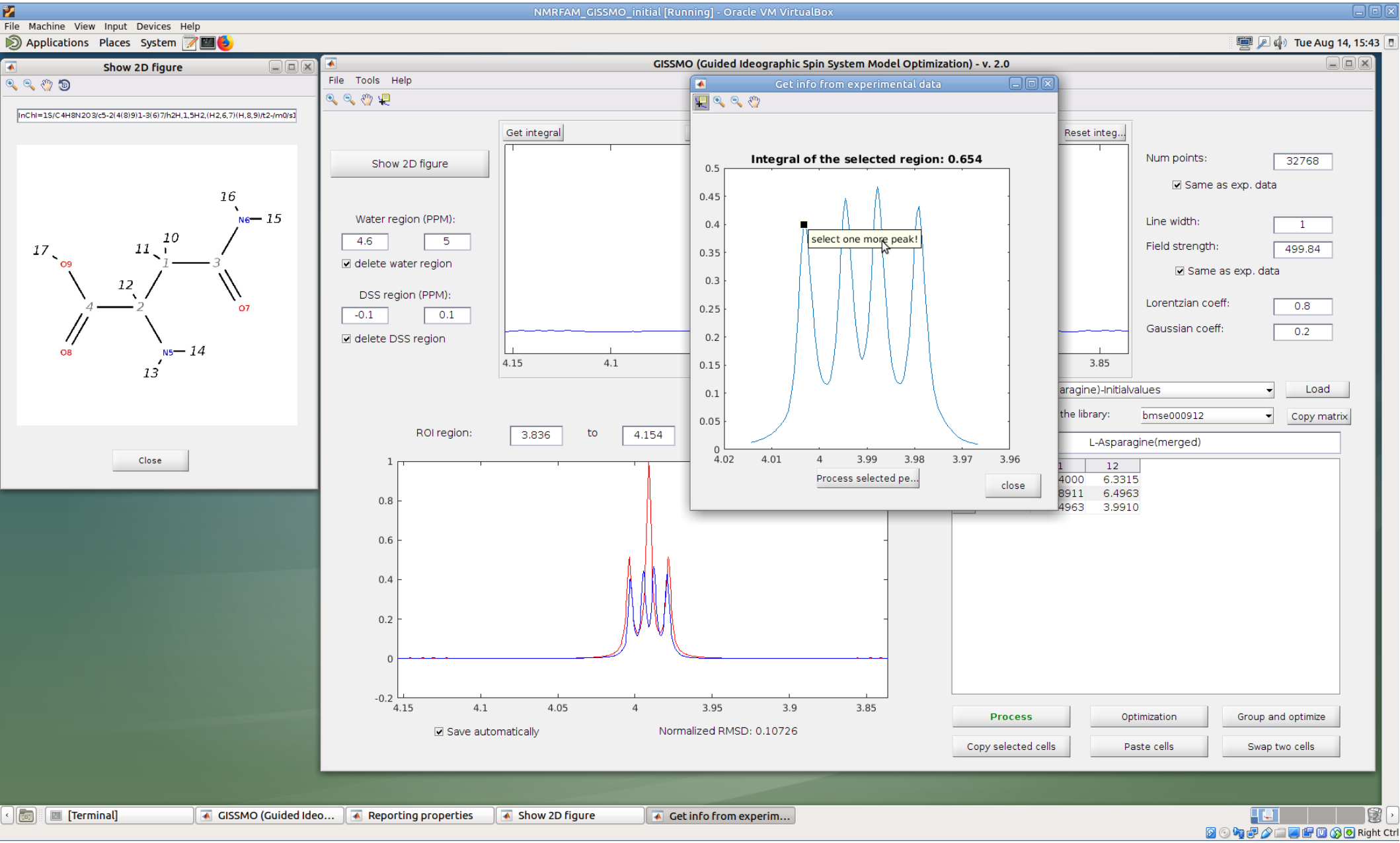
Process selected pe...

close

[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure Get info from experim...

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:43
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
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
Reset integ...
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Load
Copy matrix
the library:
bmse000912
L-Asparagine(merged)
ROI region:
3.836
to
4.154
Save automatically
Normalized RMSD: 0.10726
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Get info from experimental data
Integral of the selected region: 0.654
select one more peak!
Process selected pe...
close
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:43
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figure
Water region (PPM):
4.6
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delete water region
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-0.1
0.1
delete DSS region
Get integral
Reset integ...
Num points:
32768
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Lorentzian coeff:
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Load
Copy matrix
the library:
bmse000912
L-Asparagine(merged)
ROI region:
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Process
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Process selected pe...
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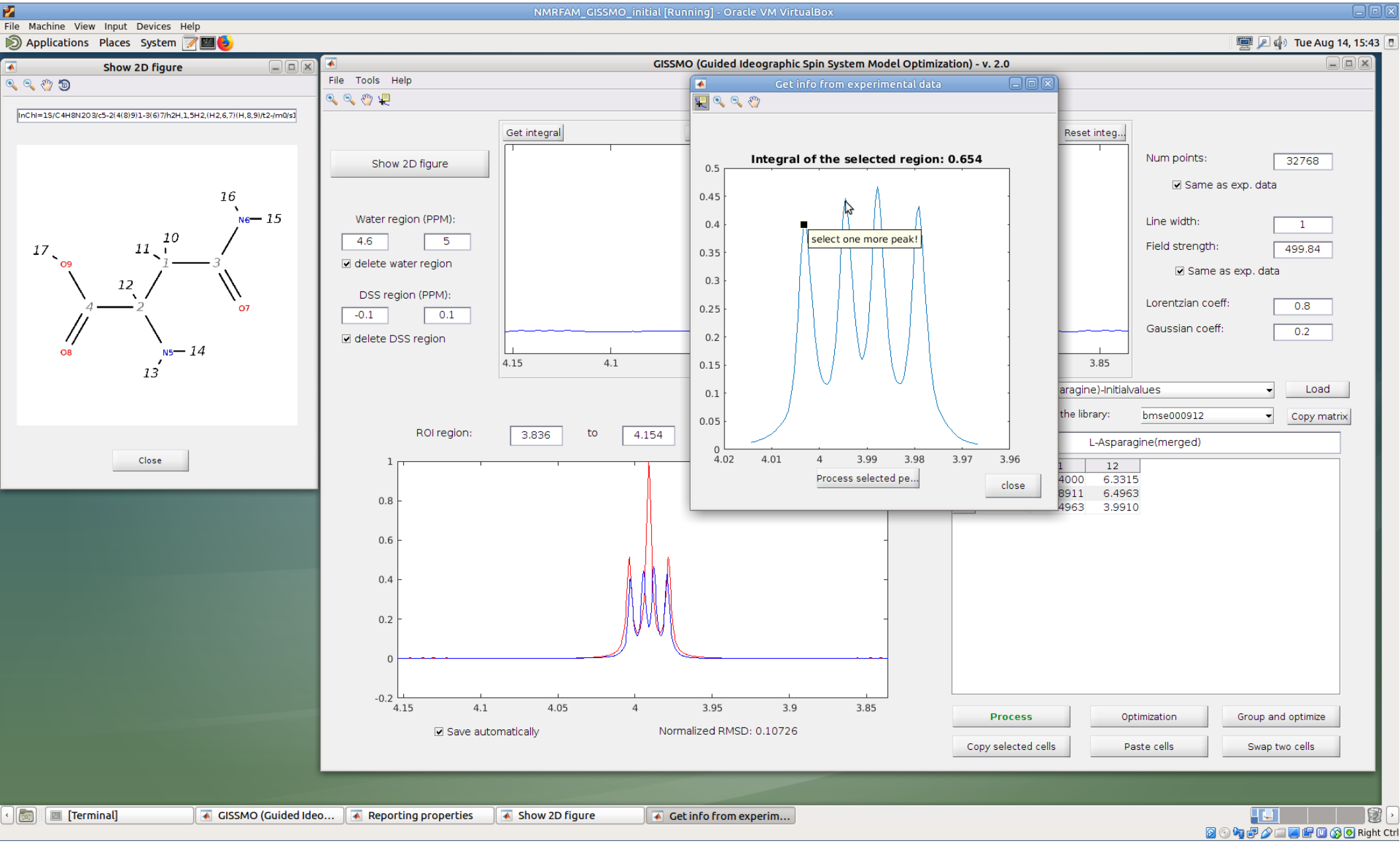
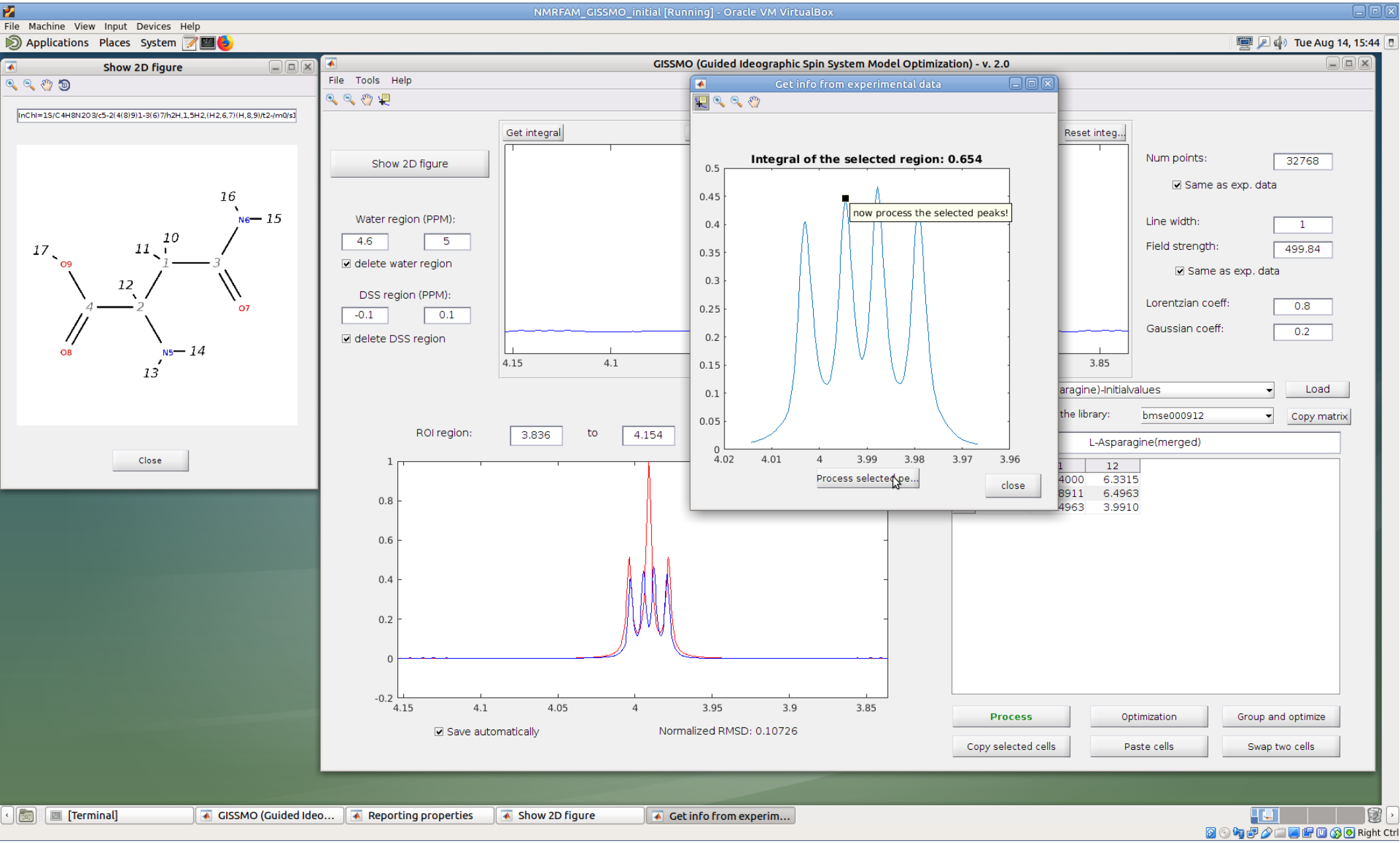
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:43
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
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
Reset integ...
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Load
Copy matrix
the library:
bmse000912
L-Asparagine(merged)
ROI region:
3.836
to
4.154
Save automatically
Normalized RMSD: 0.10726
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Get info from experimental data
Integral of the selected region: 0.654
select one more peak!
Process selected pe...
close
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:44
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
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
Reset integ...
ROI region:
3.836
to
4.154
Save automatically
Normalized RMSD: 0.10726
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
Load
the library:
bmse000912
Copy matrix
L-Asparagine(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Get info from experimental data
Integral of the selected region: 0.654
now process the selected peaks!
Process selected pe...
close
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

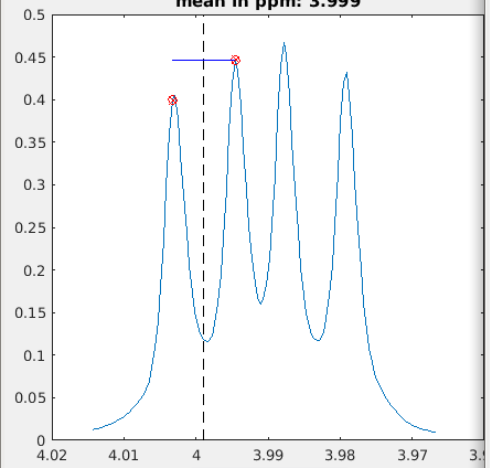
Tue Aug 14, 15:45

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

Get info from experimental data

Integral of the selected region: 0.654
difference in Hz: 4.360
mean in ppm: 3.999

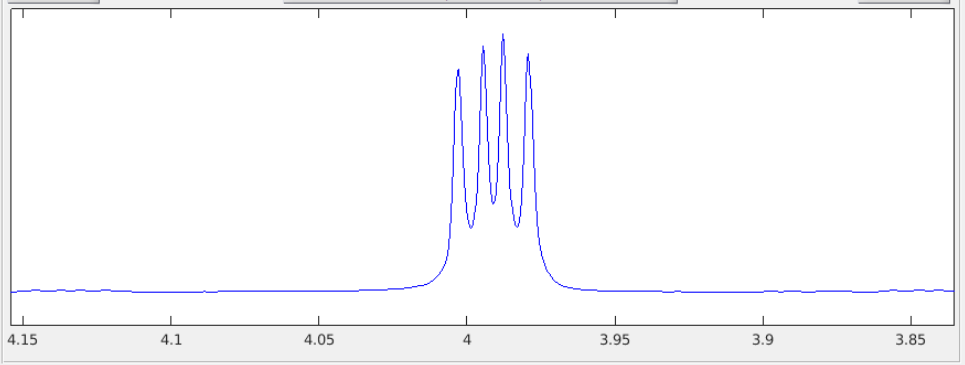


Process selected pe...

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

☑ delete water region

DSS region (PPM): -0.1 0.1

☑ delete DSS region

Num points: 32768

☑ Same as exp. data

Line width: 1

Field strength: 499.84

☑ Same as exp. data

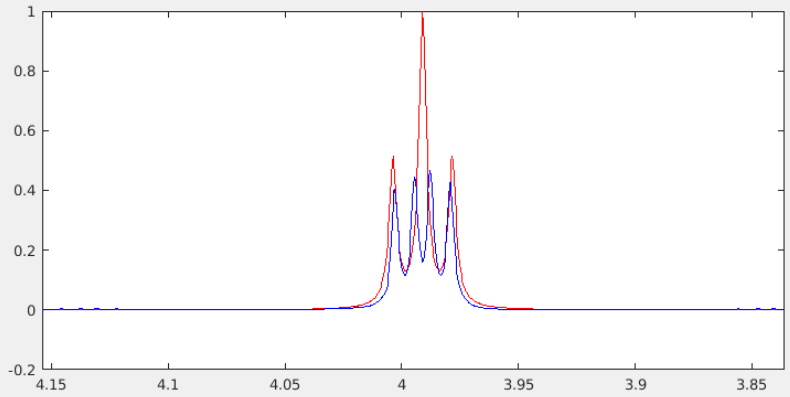
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 3.836 to 4.154 get ROI from exp. spectrum



☑ Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.36
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Get info from experim...

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

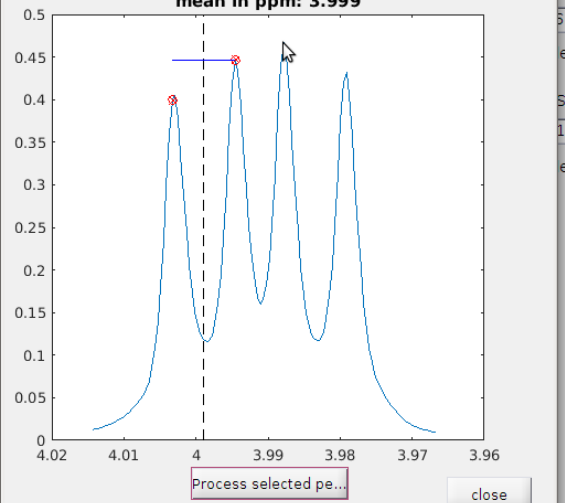
Tue Aug 14, 15:45

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

Get info from experimental data

Integral of the selected region: 0.654
difference in Hz: 4.360
mean in ppm: 3.999



Process selected pe...

close

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

File Tools Help

Show 2D figure

ter region (PPM):

5

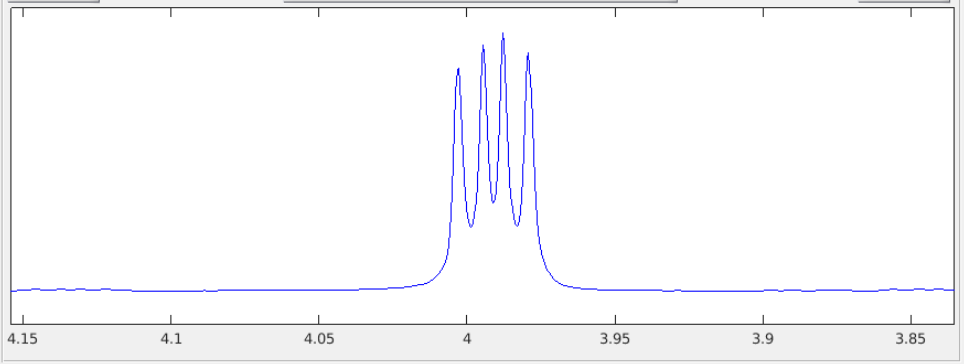
ete water region

SS region (PPM):

0.1

ete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

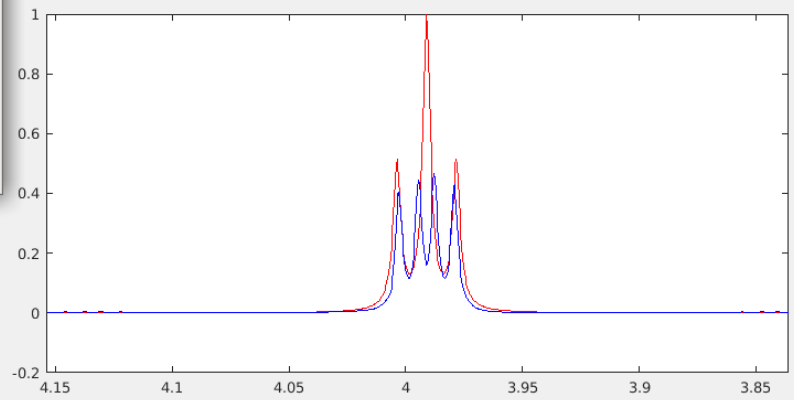
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

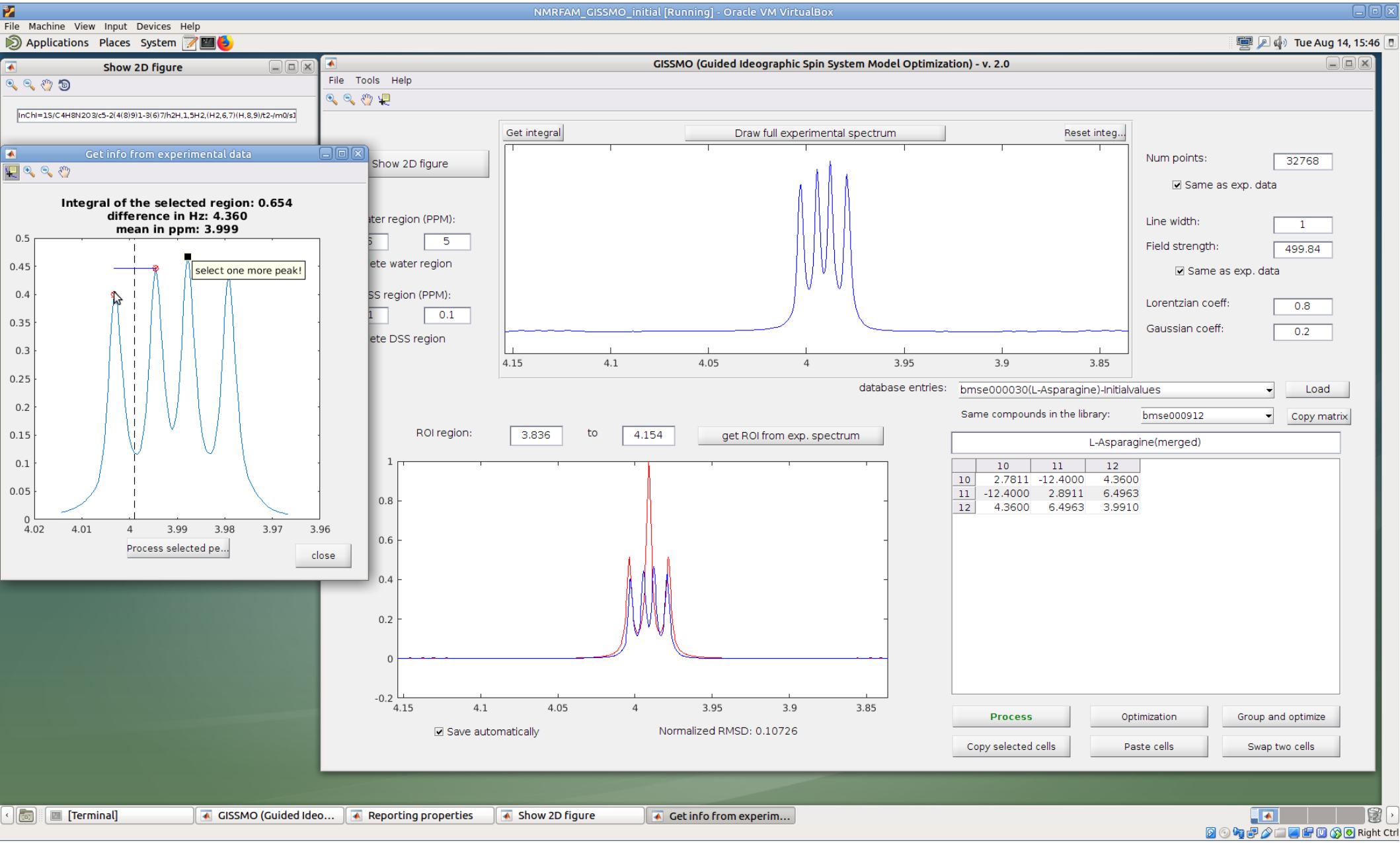
	10	11	12
10	2.7811	-12.4000	4.36
11	-12.4000	2.8911	6.4963
12	6.3315	6.4963	3.9910

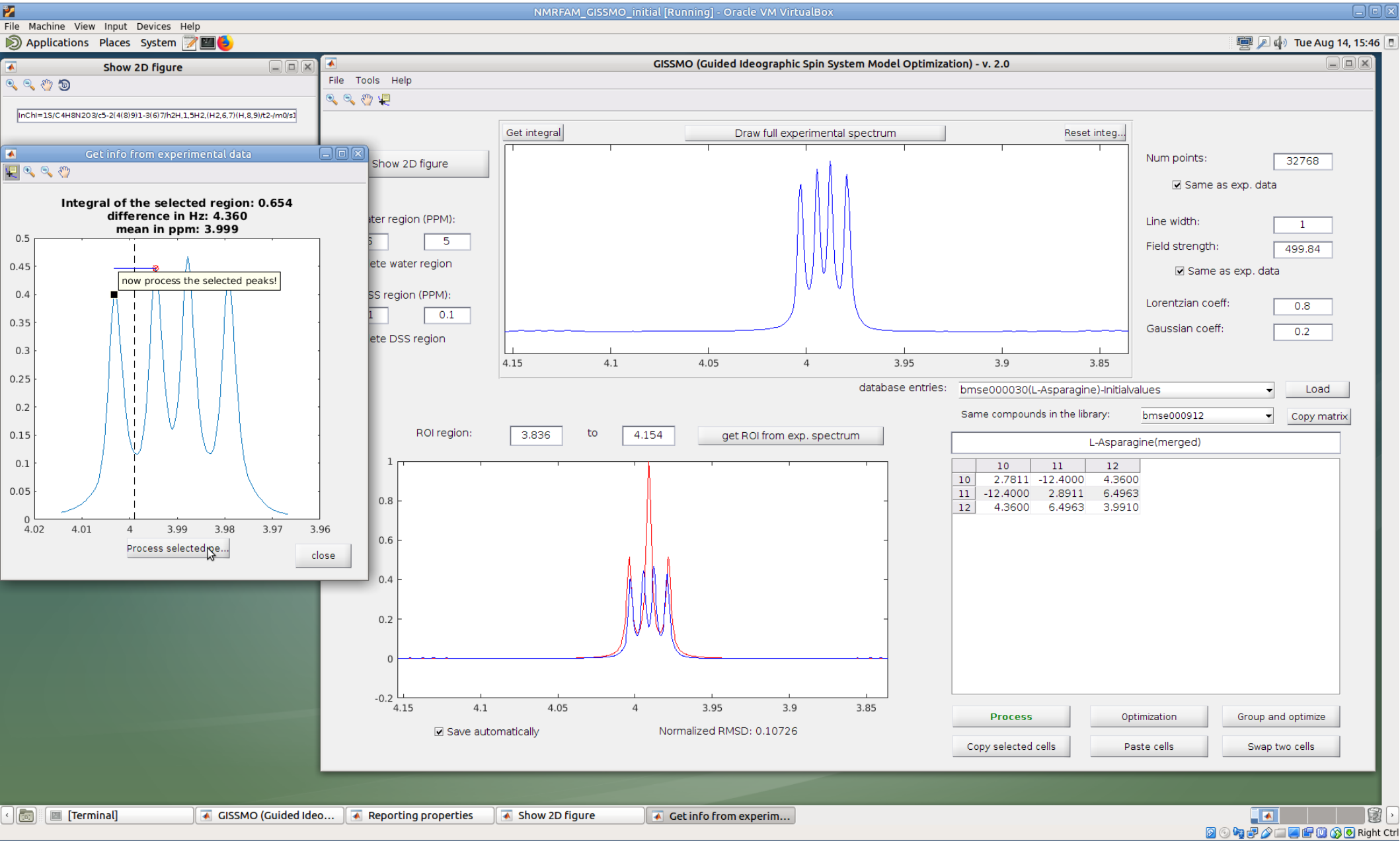
Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Get info from experim...

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:46
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
Get info from experimental data
Integral of the selected region: 0.654
difference in Hz: 4.360
mean in ppm: 3.999
select one more peak!
Process selected pe...
close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
ter region (PPM):
5
ete water region
SS region (PPM):
0.1
ete 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:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
3.836
to
4.154
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.7811 -12.4000 4.3600
11 -12.4000 2.8911 6.4963
12 4.3600 6.4963 3.9910
Save automatically
Normalized RMSD: 0.10726
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 15:46
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
Get info from experimental data
Integral of the selected region: 0.654
difference in Hz: 4.360
mean in ppm: 3.999
now process the selected peaks!
Process selected pe...
close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figure
Get integral
Draw full experimental spectrum
Reset integ...
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
ter region (PPM):
5
ete water region
SS region (PPM):
0.1
ete DSS region
database entries:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
3.836
to
4.154
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.7811 -12.4000 4.3600
11 -12.4000 2.8911 6.4963
12 4.3600 6.4963 3.9910
Save automatically
Normalized RMSD: 0.10726
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Get info from experim...
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

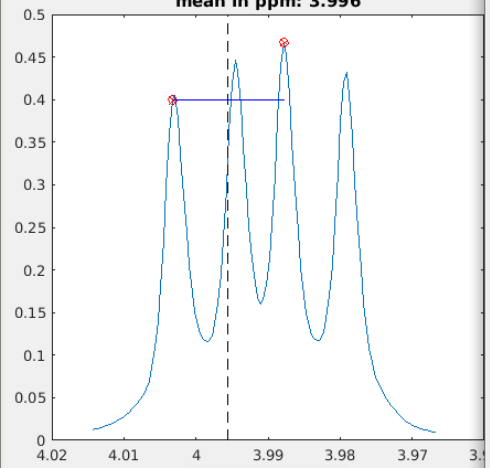
Tue Aug 14, 15:46

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

Get info from experimental data

Integral of the selected region: 0.654
difference in Hz: 7.728
mean in ppm: 3.996

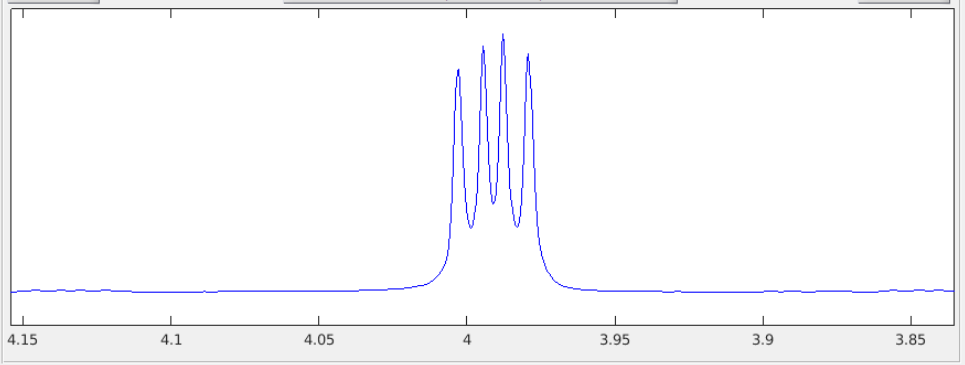


Process selected pe...

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

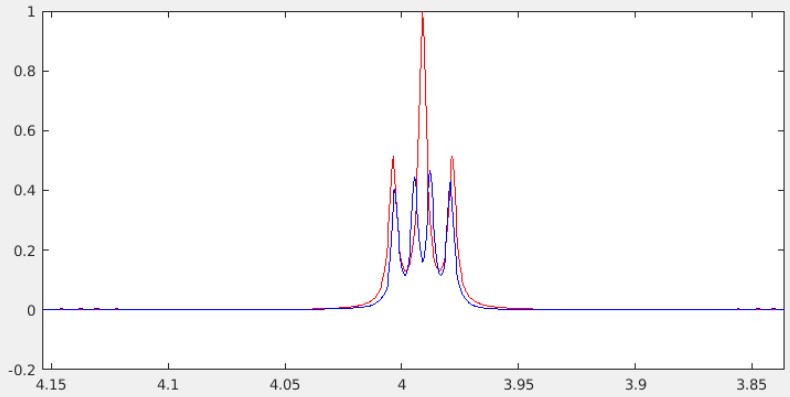
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 3.836 to 4.154 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	6.4963
12	4.3600	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Get info from experim...

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

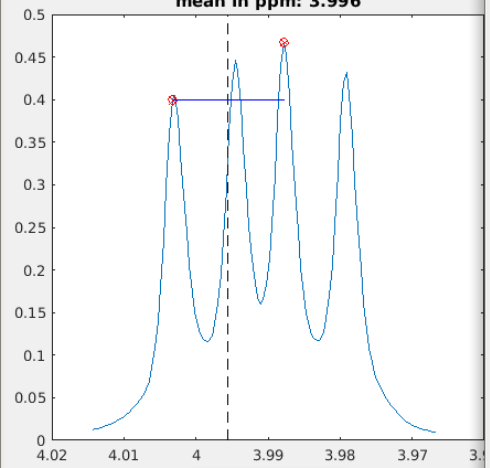
Tue Aug 14, 15:47

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

Get info from experimental data

Integral of the selected region: 0.654
difference in Hz: 7.728
mean in ppm: 3.996

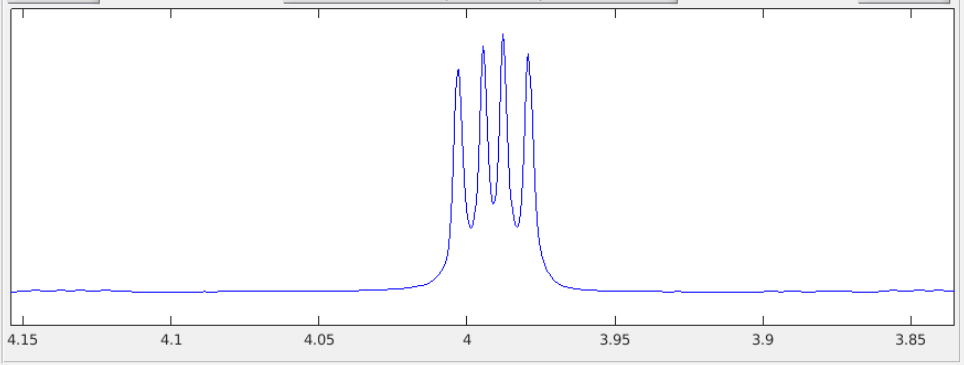


Process selected pe...

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

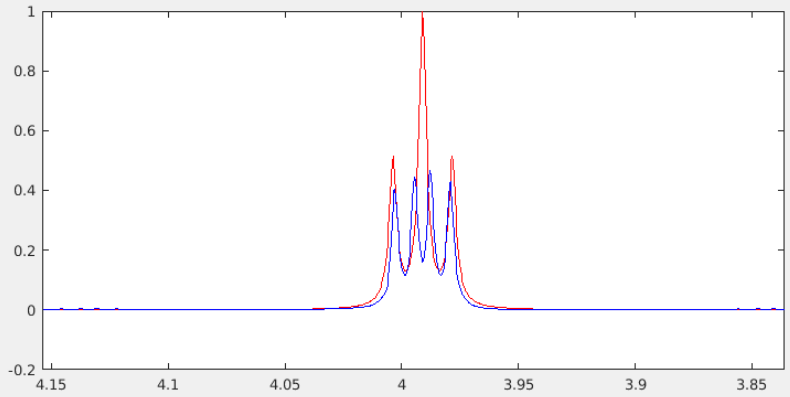
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 3.836 to 4.154 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.728
12	4.3600	6.4963	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Get info from experim...

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

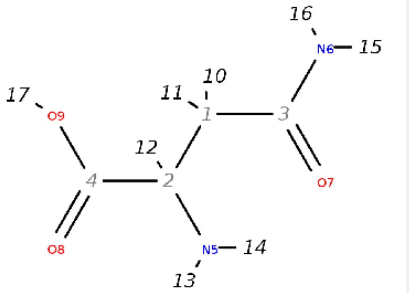
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:47

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

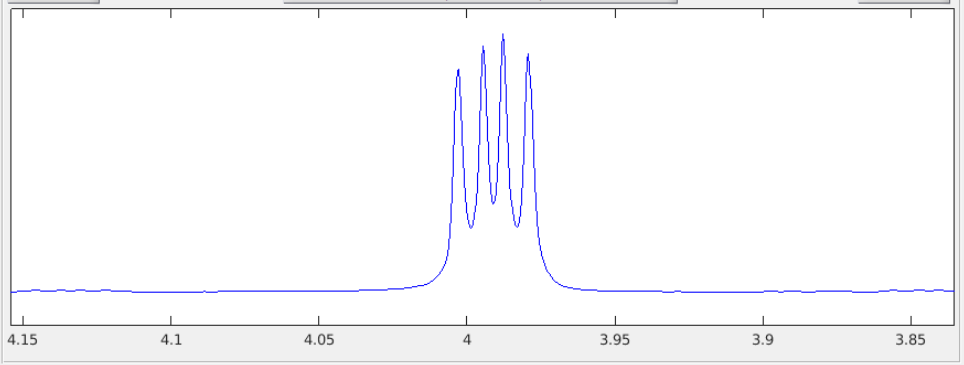
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

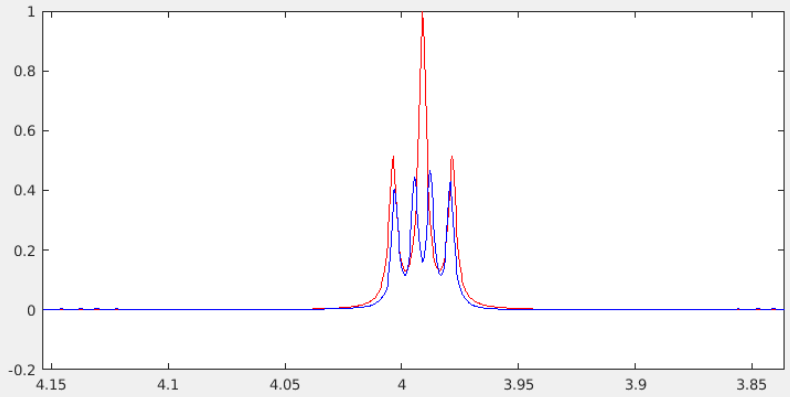
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10726

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
12	4.3600	7.7280	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

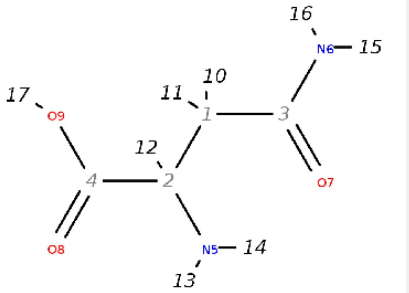
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:48

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

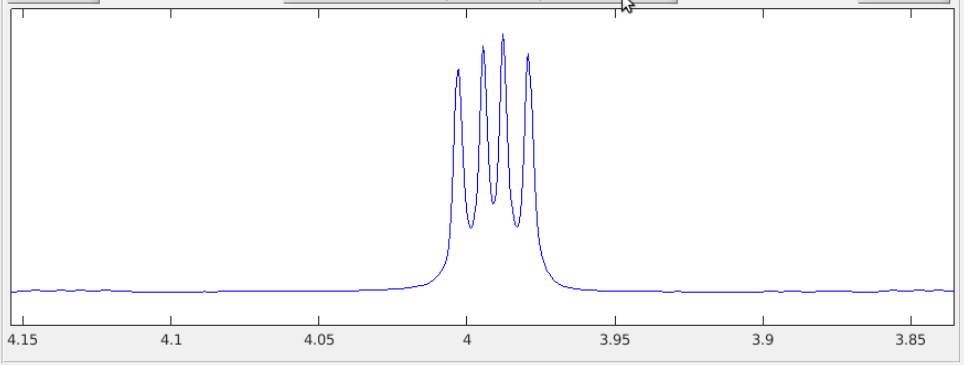
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

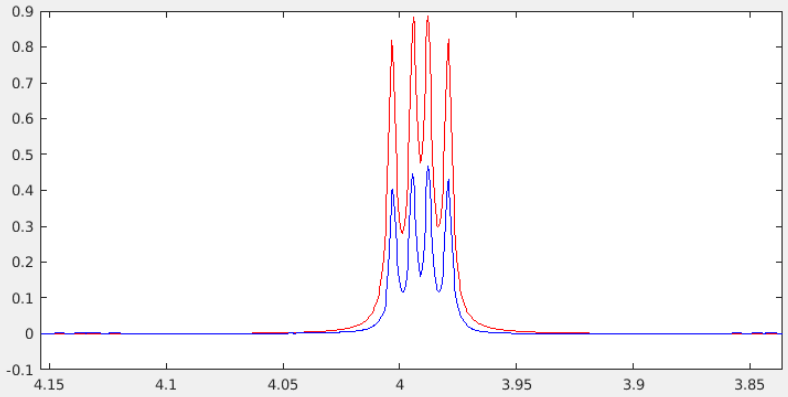
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
12	4.3600	7.7280	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

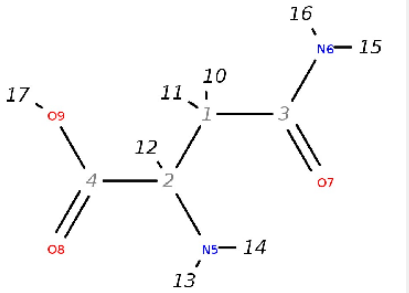
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:48

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

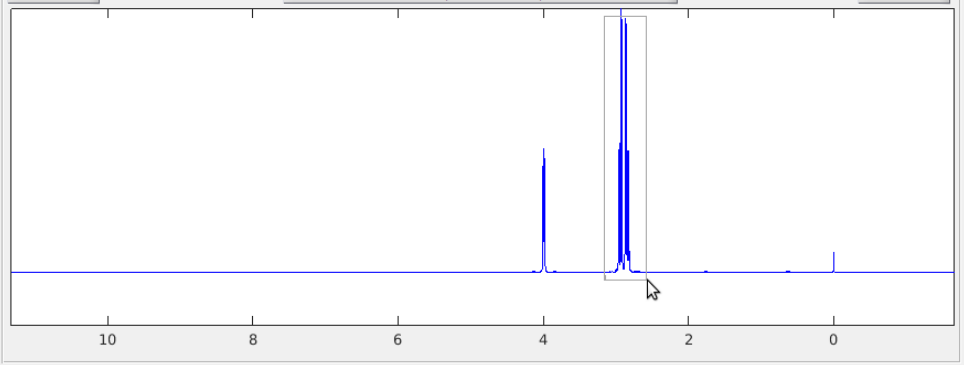
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

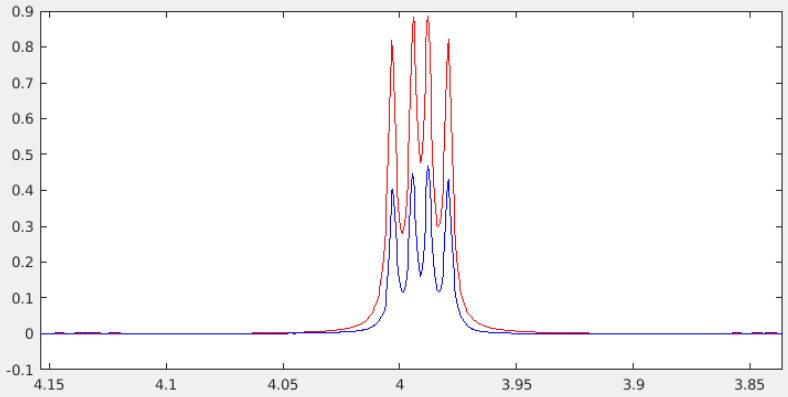
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
12	4.3600	7.7280	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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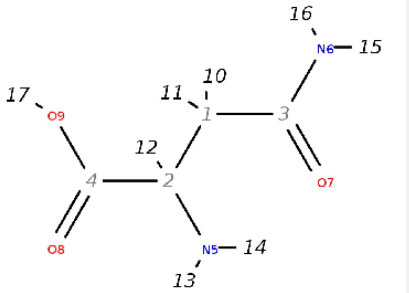
Applications Places System

Tue Aug 14, 15:48

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

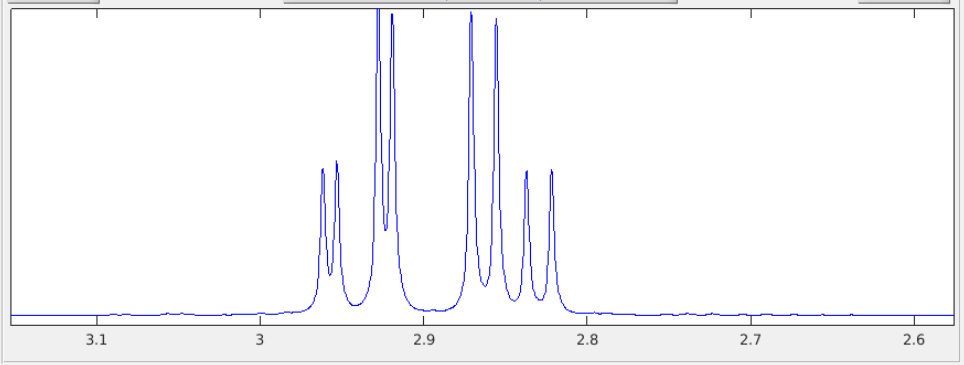
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

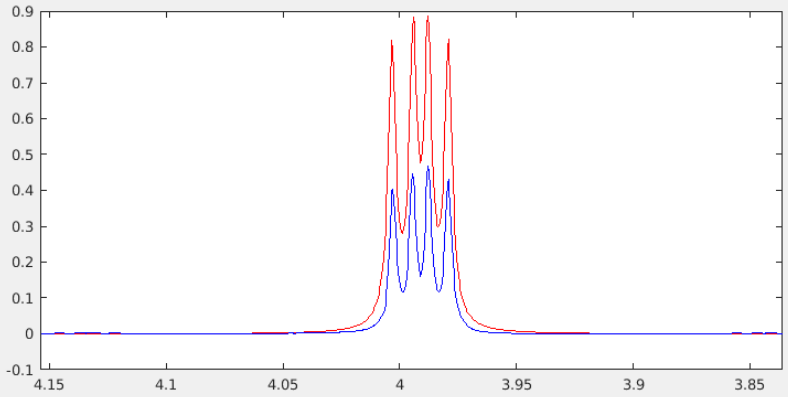
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 3.836 to 4.154 | get ROI from exp. spectrum



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	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
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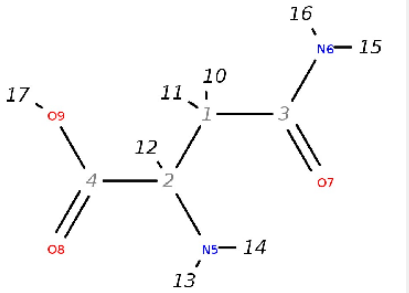
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:49

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



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

File Tools Help

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delete water region

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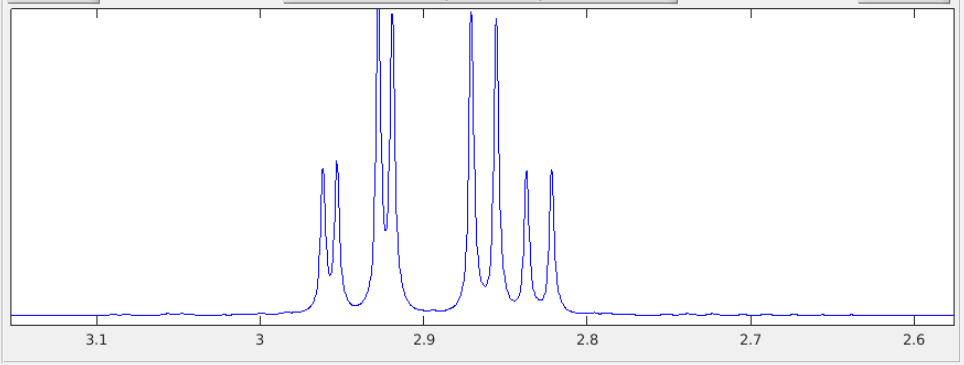

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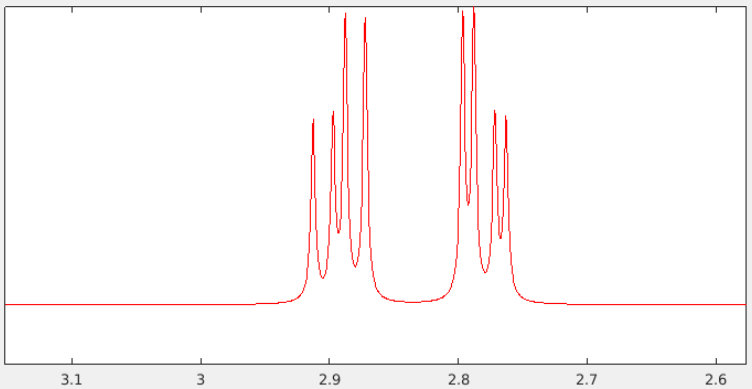
database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
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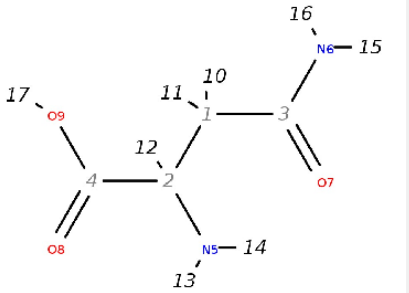
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:51

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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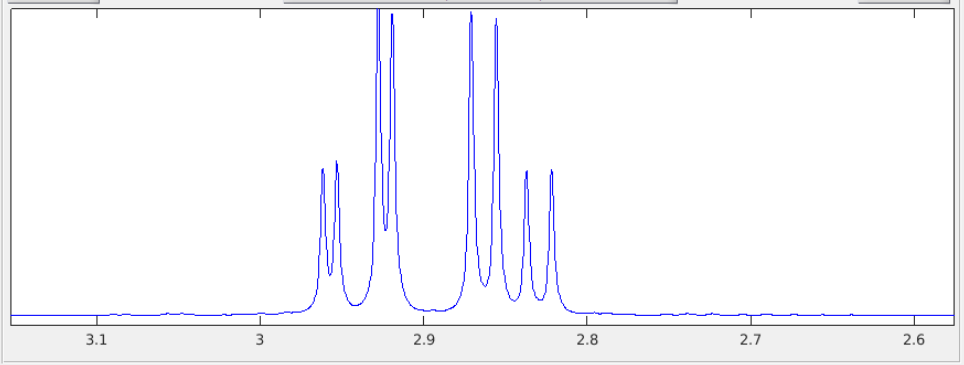

Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

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Line width: 1

Field strength: 499.84

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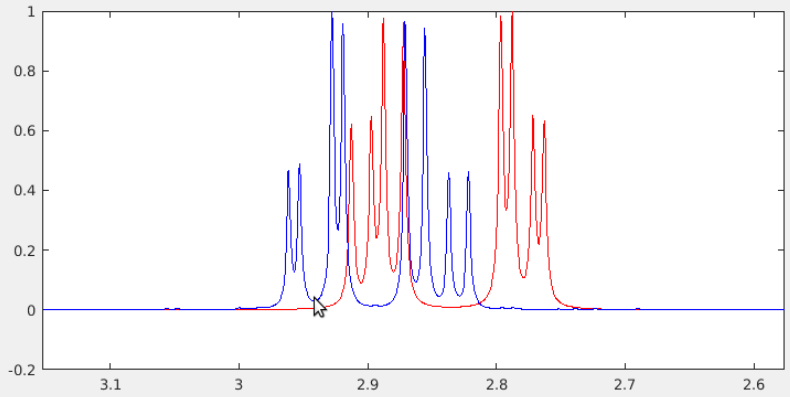

Save automatically

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L-Asparagine(merged)

	10	11	12
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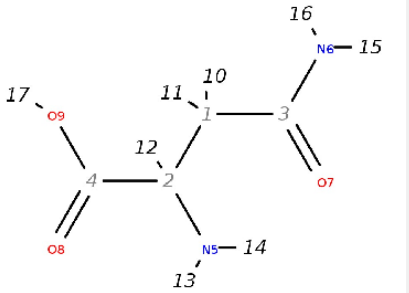
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



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

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Water region (PPM): 4.6 5

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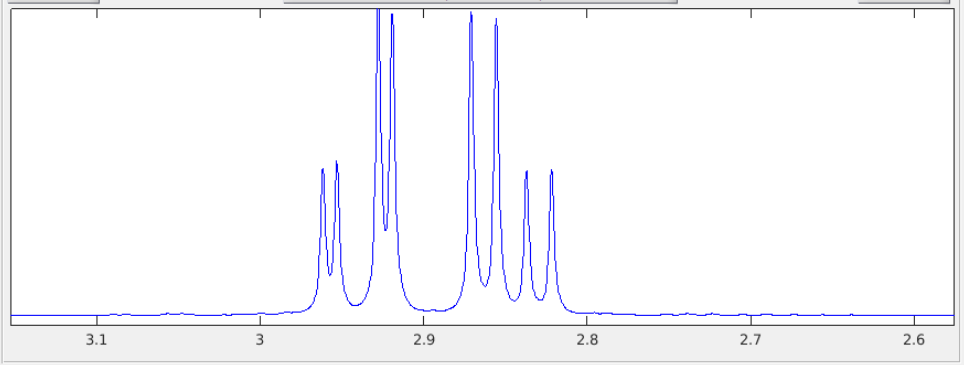

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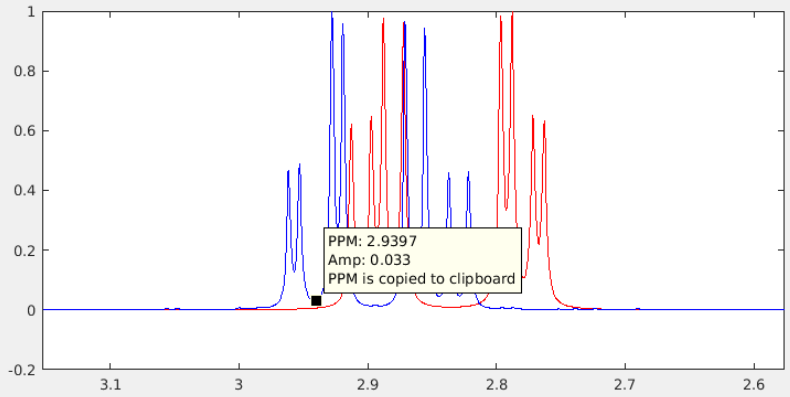

Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.8911	7.7280
12	4.3600	7.7280	3.9910

Process | Optimization | Group and optimize

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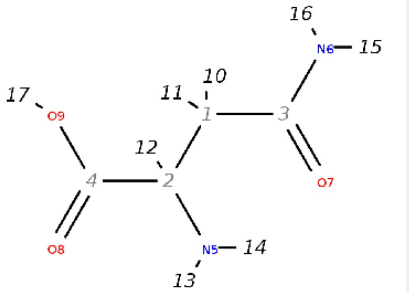
Applications Places System

Tue Aug 14, 15:52

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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Water region (PPM): 4.6 5

delete water region

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delete DSS region

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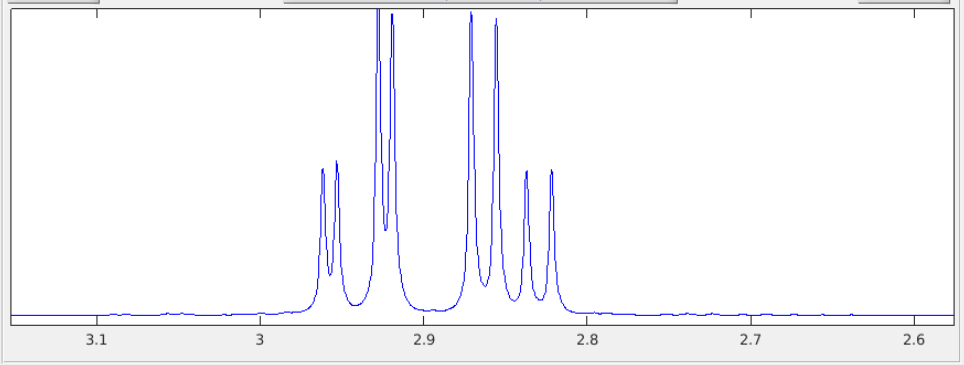


Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

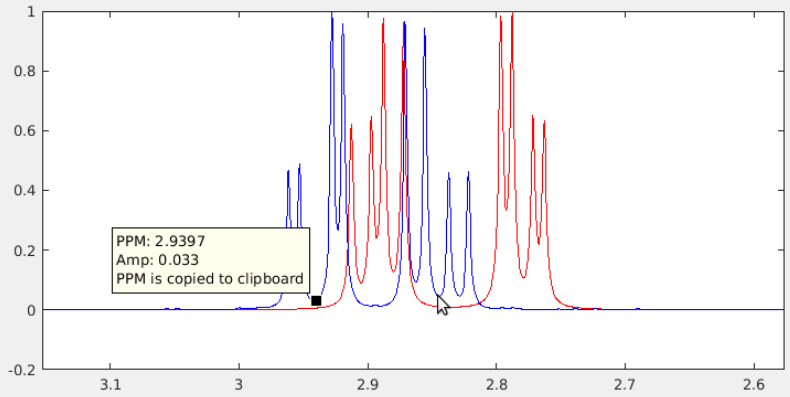
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.9397	7.7280
12	4.3600	7.7280	3.9910

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File Machine View Input Devices Help

Applications Places System

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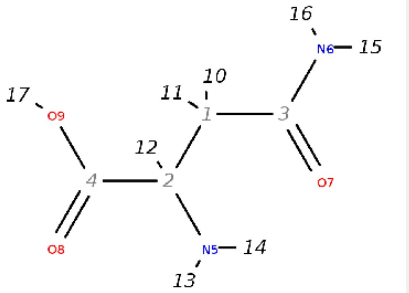
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

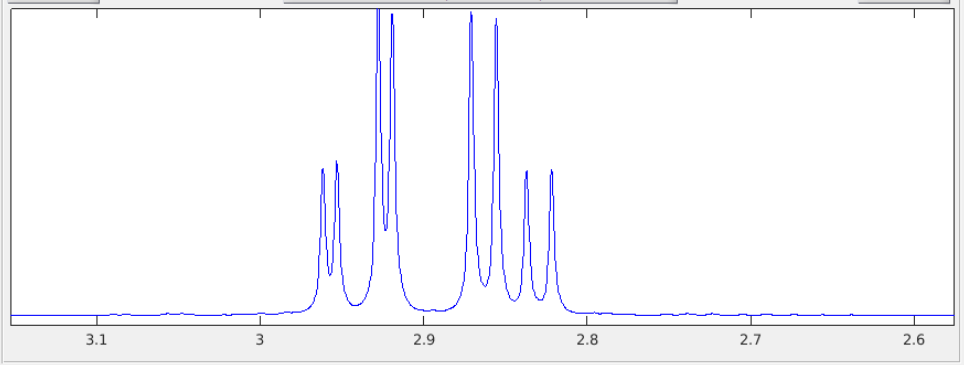


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

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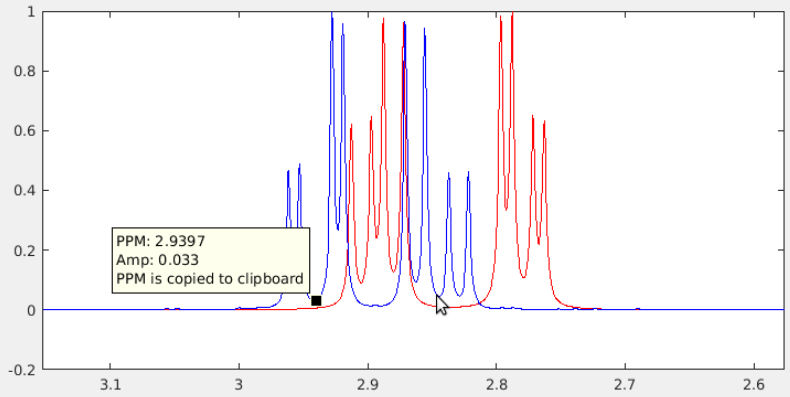
ROI region: 2.576 to 3.153 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.7811	-12.4000	4.3600
11	-12.4000	2.9397	7.7280
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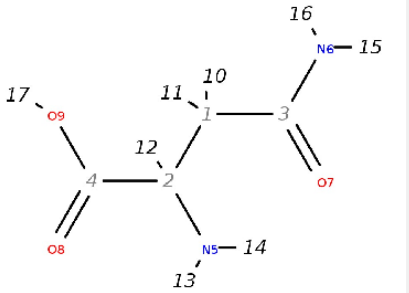

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GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0

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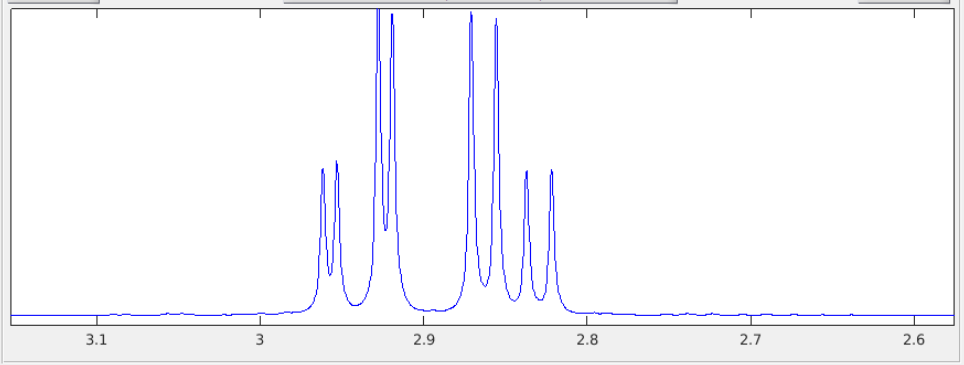

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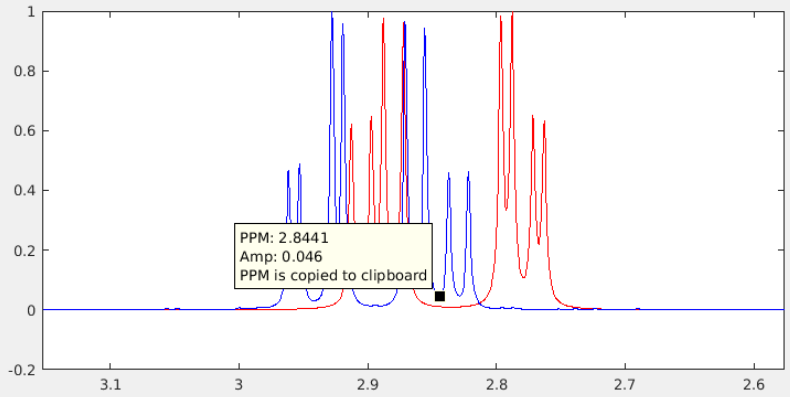

Save automatically

Normalized RMSD: 0.09815

L-Asparagine(merged)

	10	11	12
10	2.8441	-12.4000	4.3600
11	-12.4000	2.9397	7.7280
12	4.3600	7.7280	3.9910

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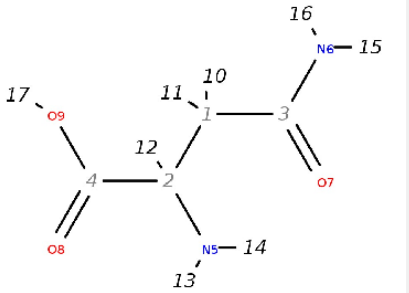
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



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

File Tools Help

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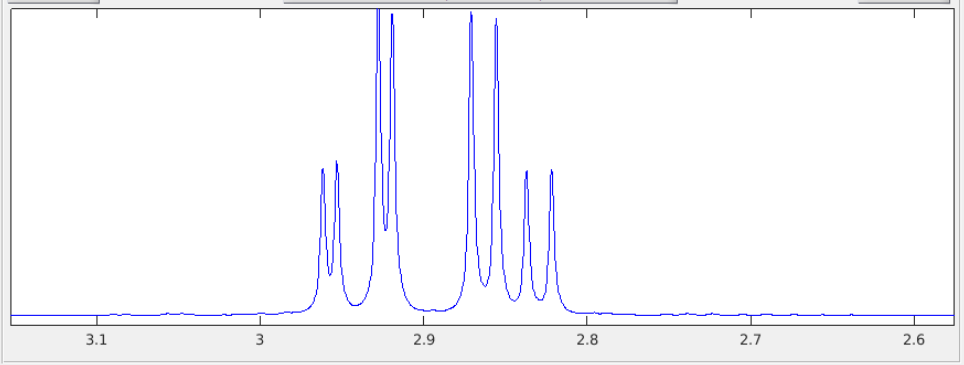

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Same as exp. data

Lorentzian coeff: 0.8

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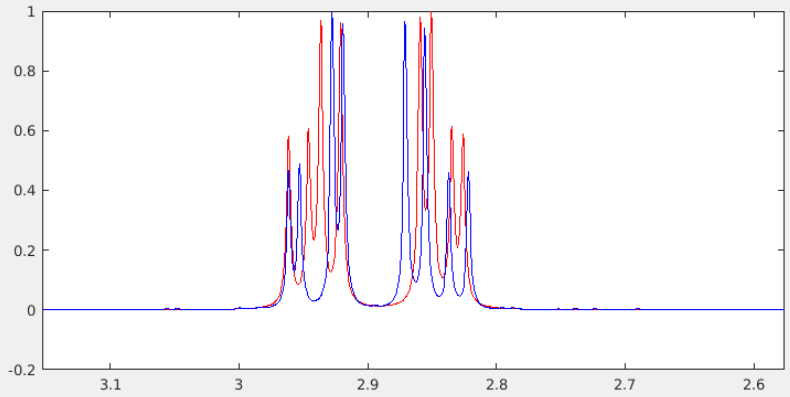
database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07776

L-Asparagine(merged)

	10	11	12
10	2.8441	-12.4000	4.3600
11	-12.4000	2.9397	7.7280
12	4.3600	7.7280	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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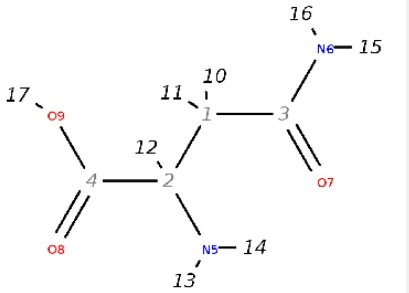
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:54

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

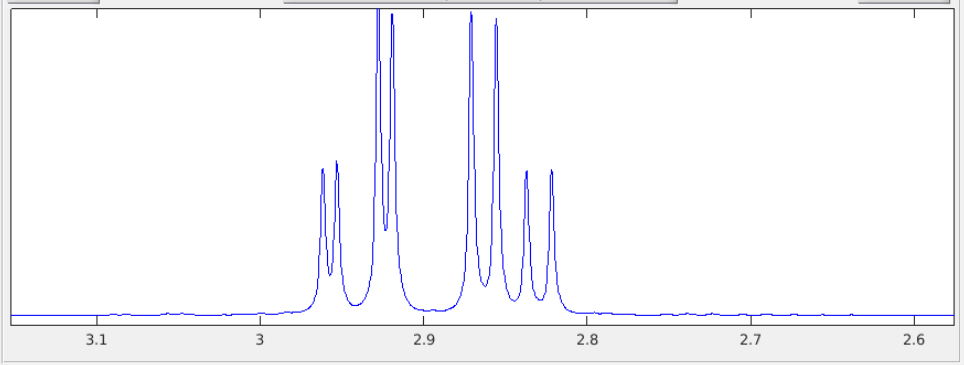
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



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Line width: 1

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Same as exp. data

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database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

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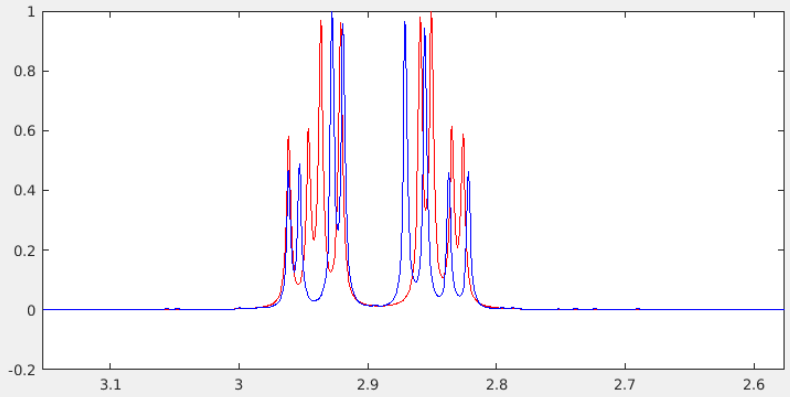

Save automatically

Normalized RMSD: 0.07776

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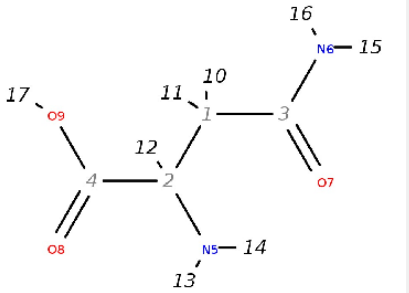
Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

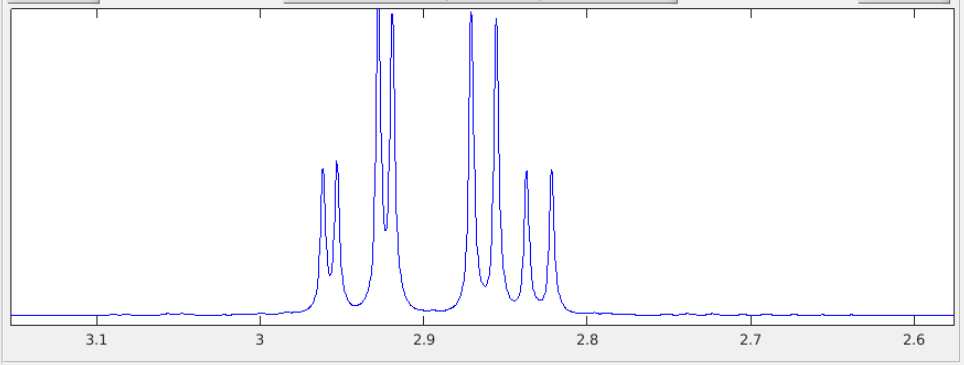
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

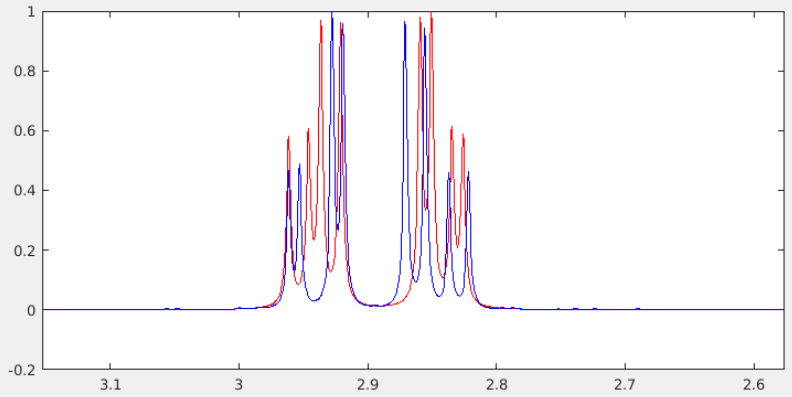
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07776

L-Asparagine(merged)

	10	11	12
10	2.8441	-12.4000	7.7280
11	-12.4000	2.9397	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

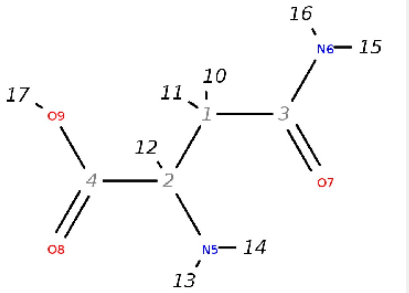
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:55

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

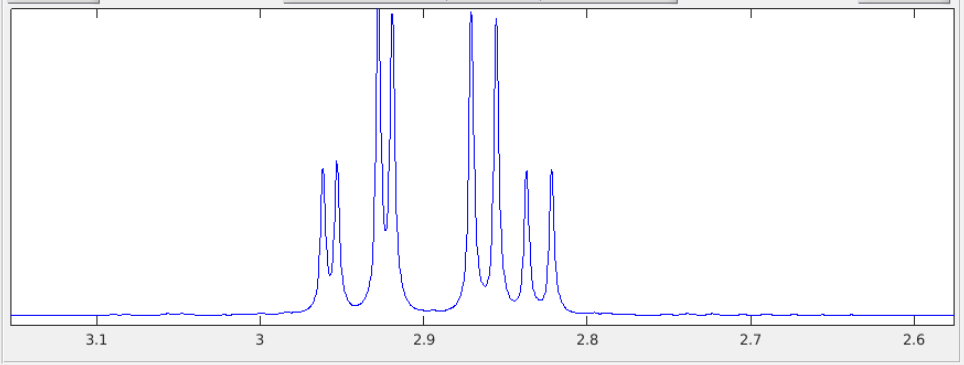
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

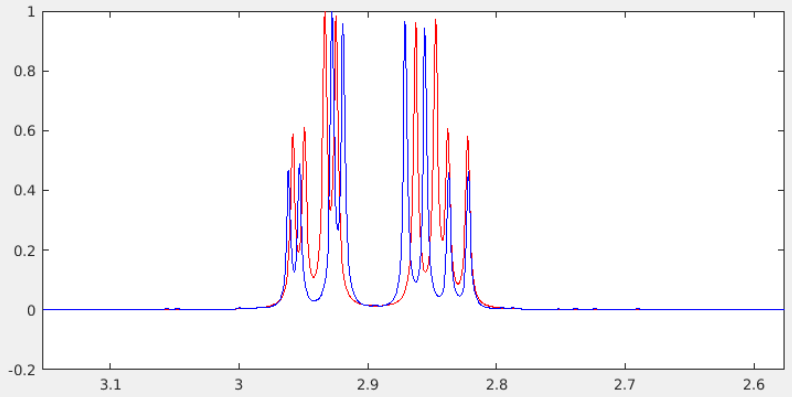
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07915

L-Asparagine(merged)

	10	11	12
10	2.8441	-12.4000	7.7280
11	-12.4000	2.9397	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

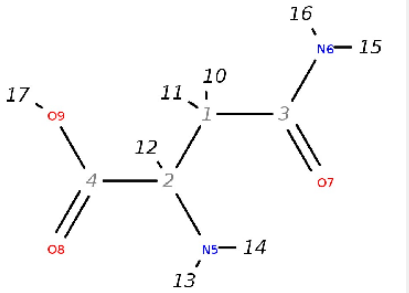
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:55

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

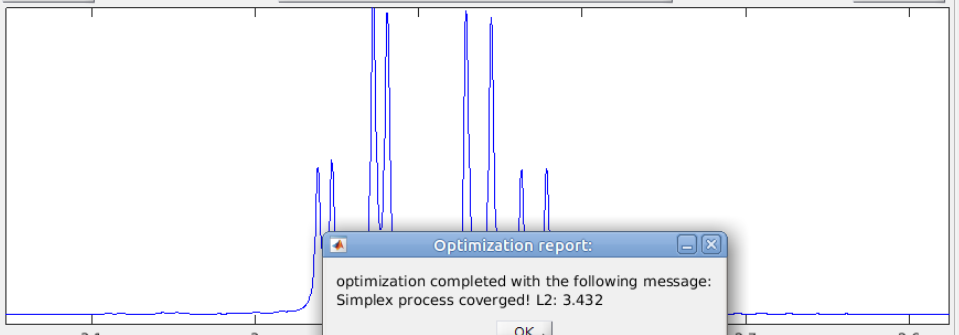
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 3.432

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

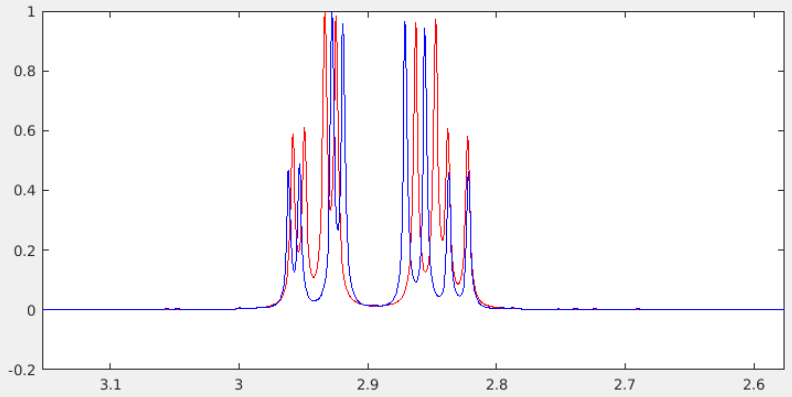
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07915

L-Asparagine(merged)

	10	11	12
10	2.8441	-23.1183	7.7280
11	-23.1183	2.9397	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

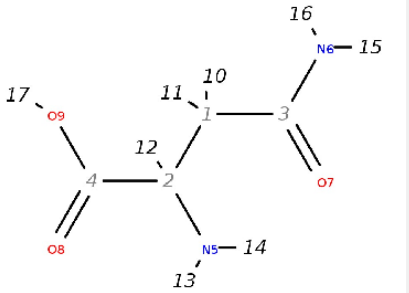
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:55

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

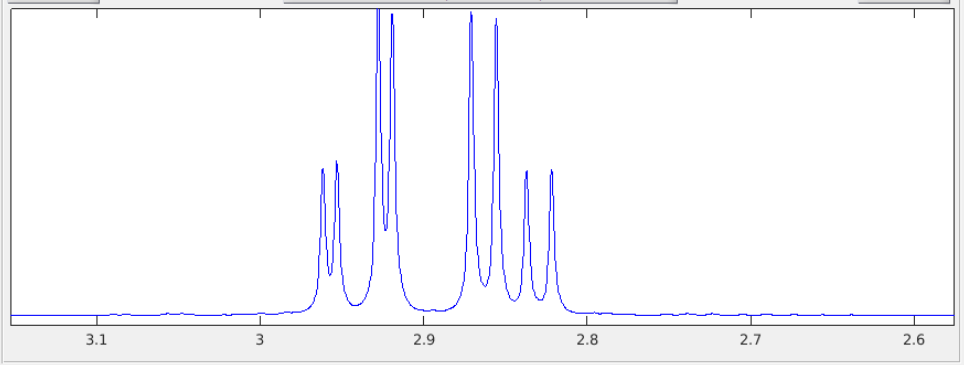
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

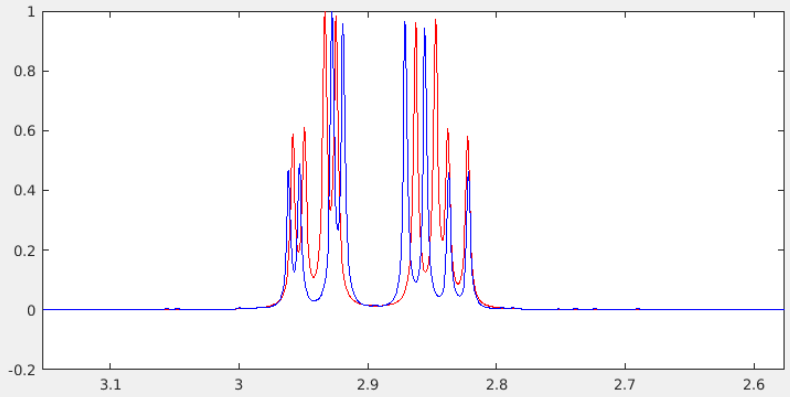
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07915

L-Asparagine(merged)

	10	11	12
10	2.8441	-23.1183	7.7280
11	-23.1183	2.9397	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

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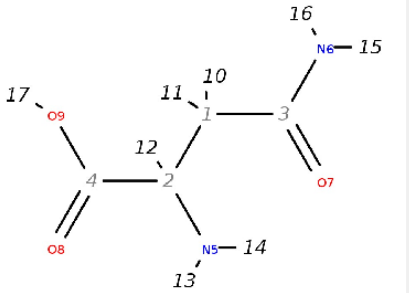
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:56

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

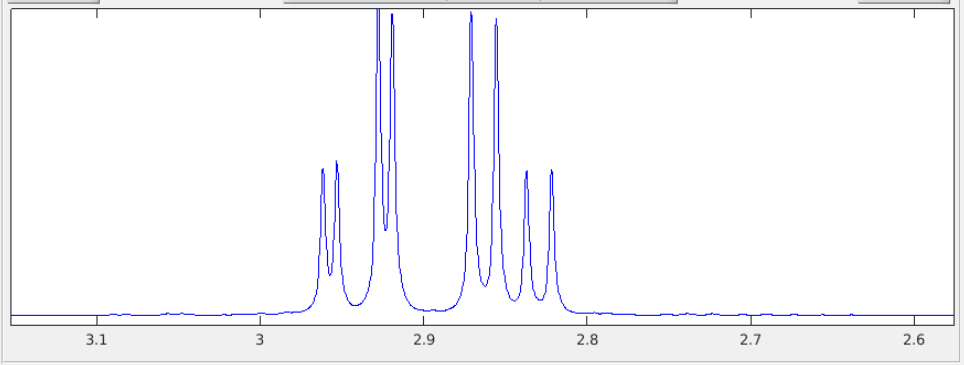
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

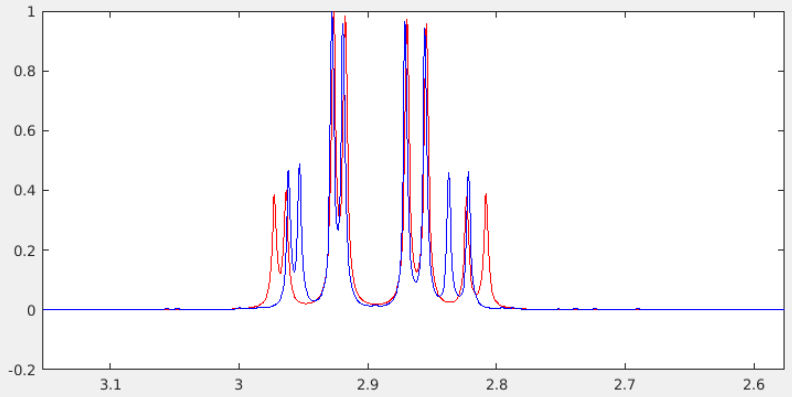
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04439

L-Asparagine(merged)

	10	11	12
10	2.8441	-23.1183	7.7280
11	-23.1183	2.9397	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

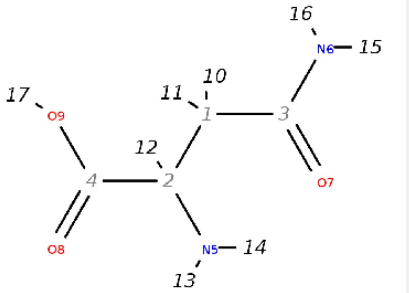
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:56

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

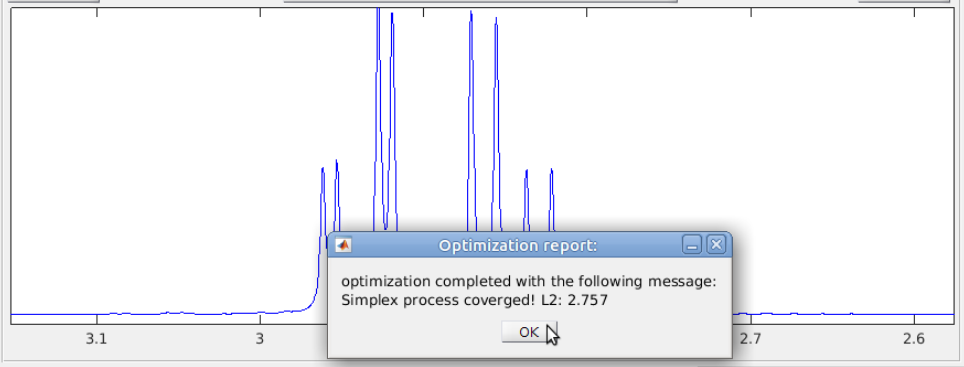
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 2.757

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

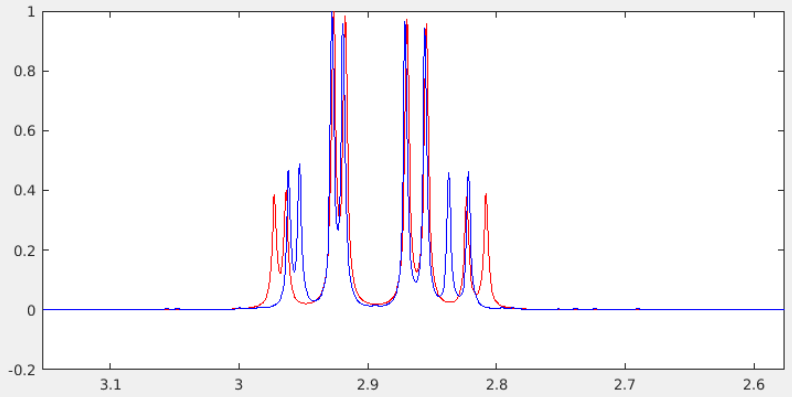
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04439

L-Asparagine(merged)

	10	11	12
10	2.8453	-23.3840	7.7280
11	-23.3840	2.9413	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

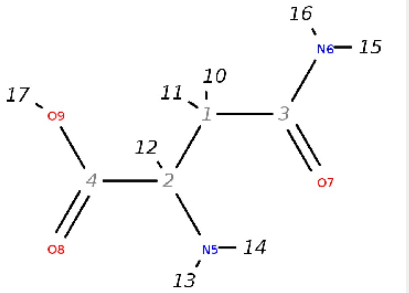
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:57

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

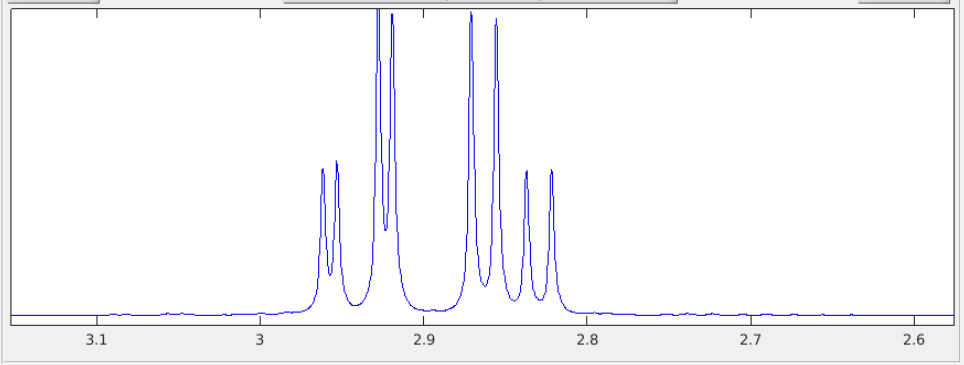
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

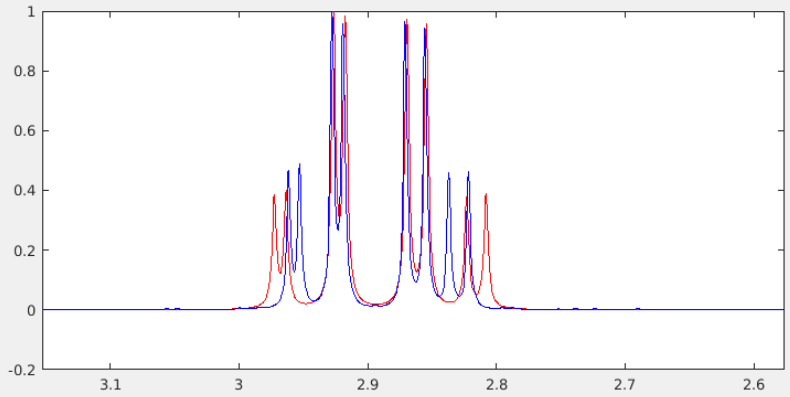
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04439

L-Asparagine(merged)

	10	11	12
10	2.8453	-23.3840	7.7280
11	-23.3840	2.9413	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

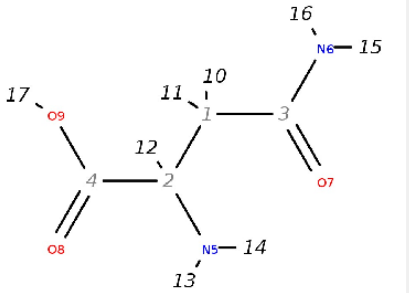
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 15:58

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

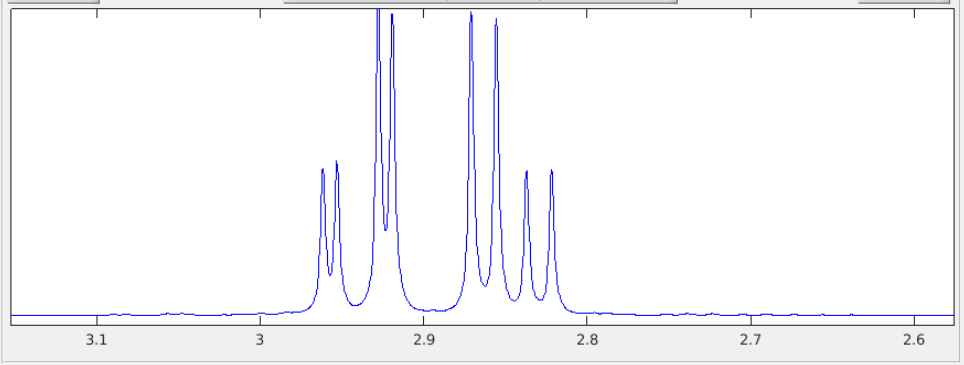
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

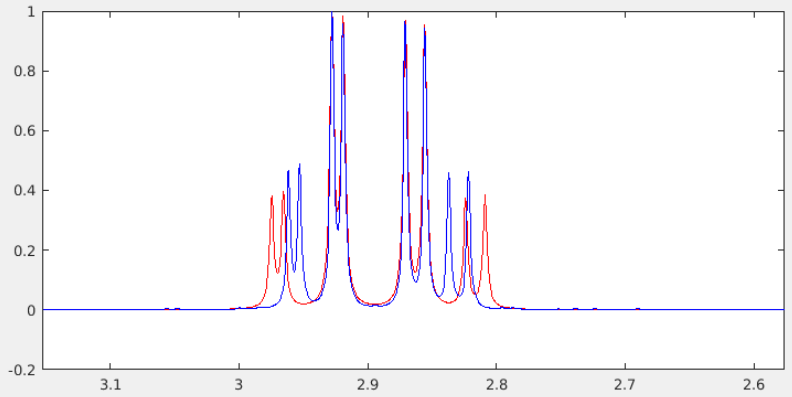
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.03631

L-Asparagine(merged)

	10	11	12
10	2.8453	-14	7.7280
11	-23.3840	2.9413	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

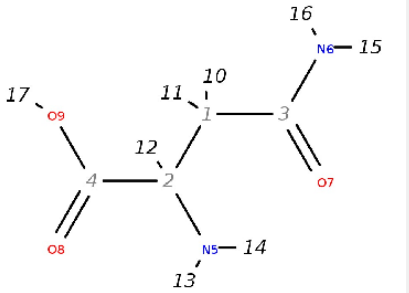
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:01

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

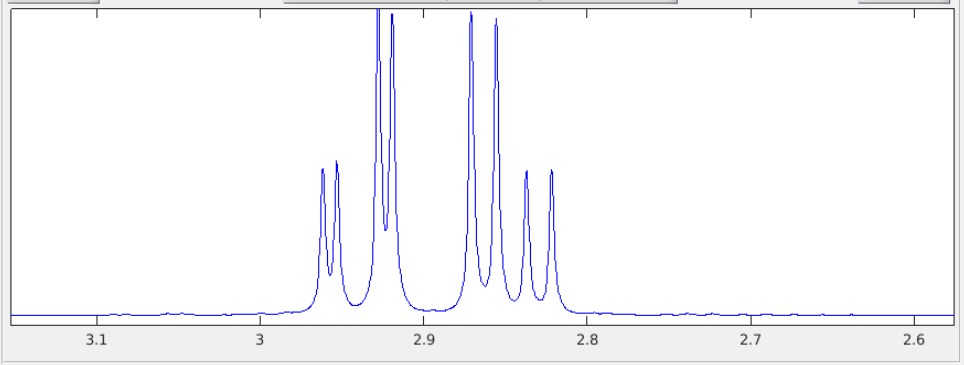
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

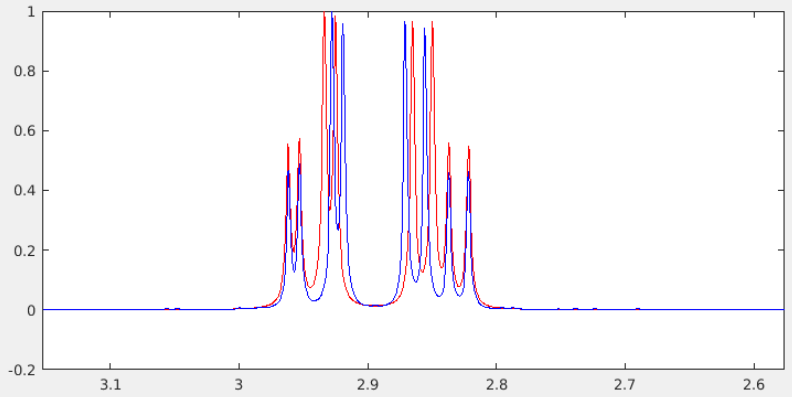
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07239

L-Asparagine(merged)

	10	11	12
10	2.8453	-14	7.7280
11	-14	2.9413	4,3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

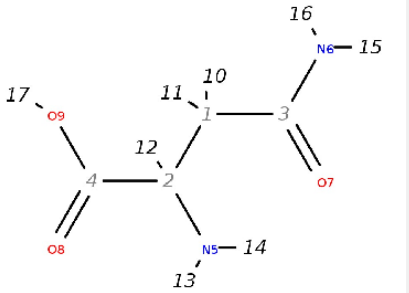
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:02

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

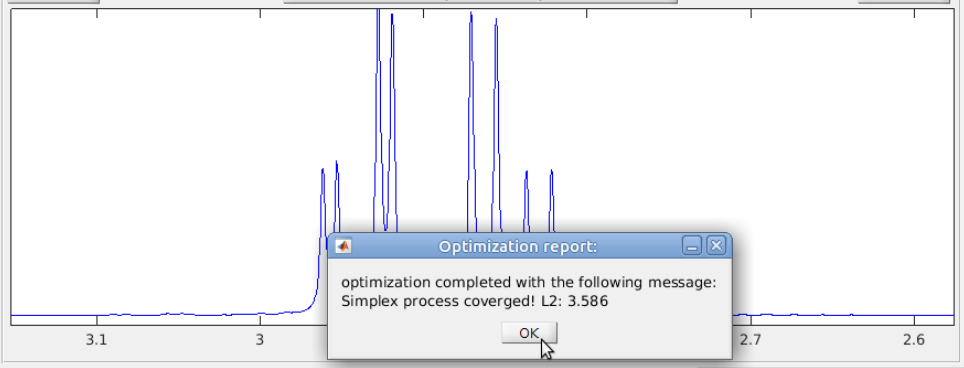
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 3.586

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

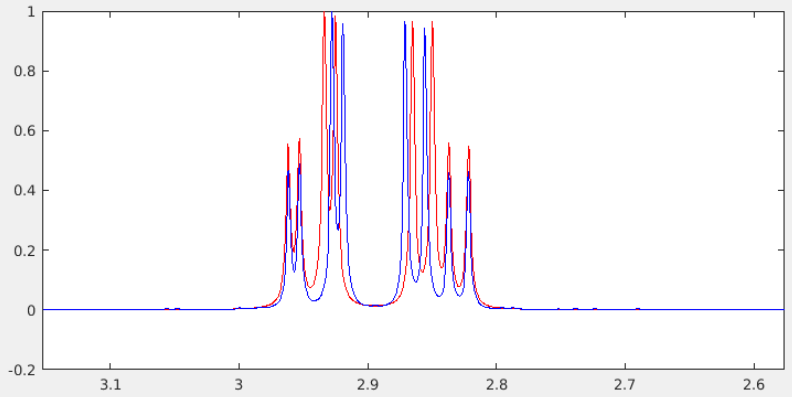
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07239

L-Asparagine(merged)

	10	11	12
10	2.8655	-16.1557	7.7280
11	-16.1557	2.9363	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

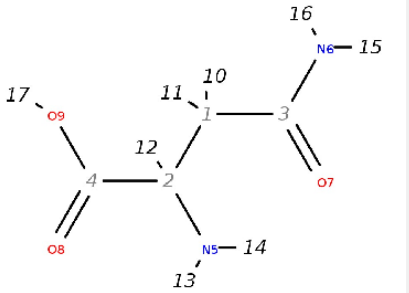
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:02

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

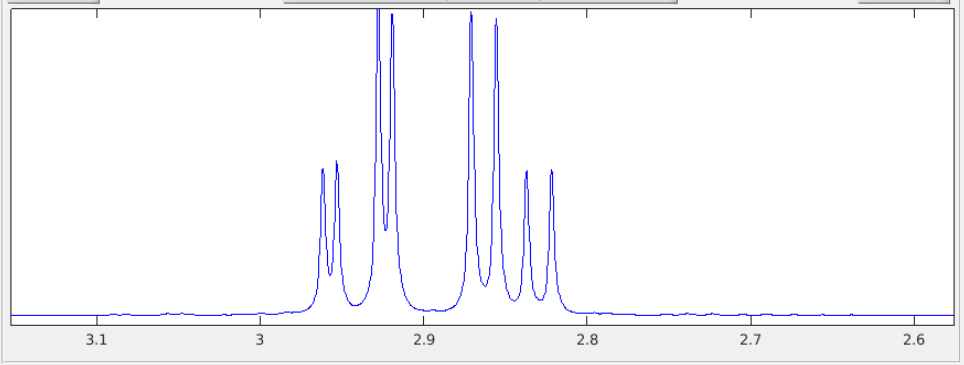
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

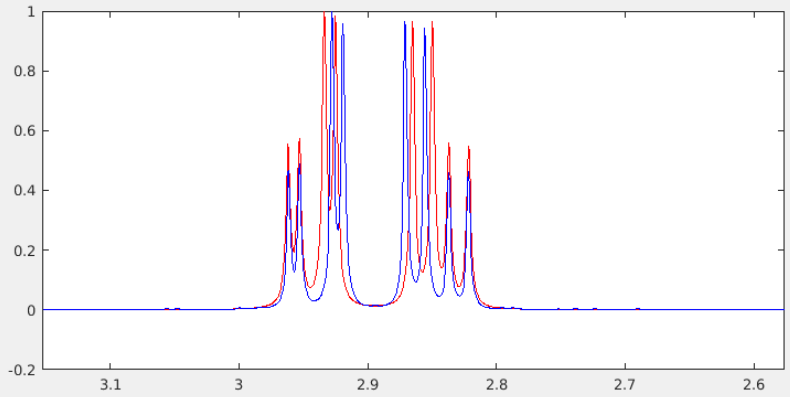
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07239

L-Asparagine(merged)

	10	11	12
10	2.8655	-16.1557	7.7280
11	-16.1557	2.9363	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

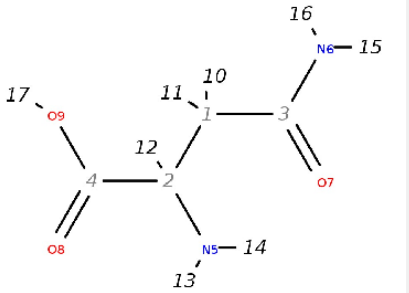
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:02

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

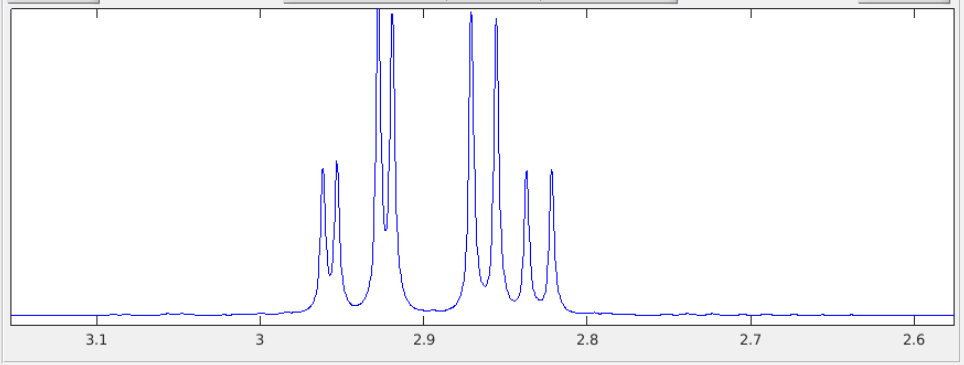
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

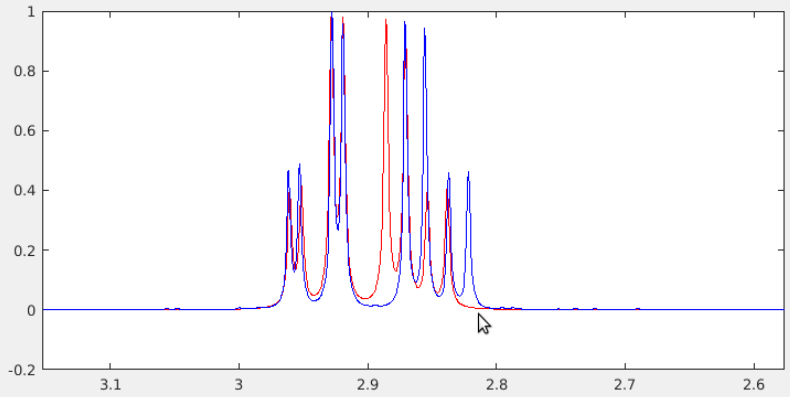
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04800

L-Asparagine(merged)

	10	11	12
10	2.8655	-16.1557	7.7280
11	-16.1557	2.9363	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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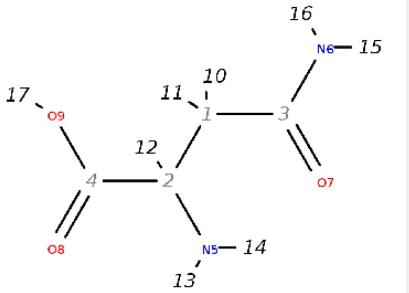
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:04

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

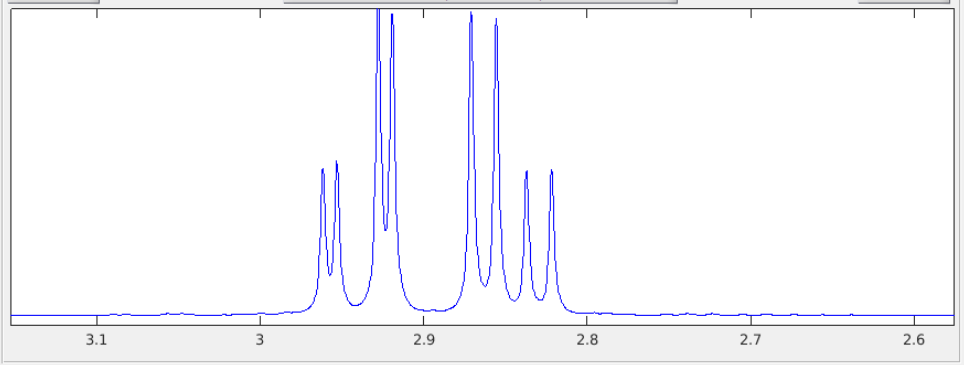
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

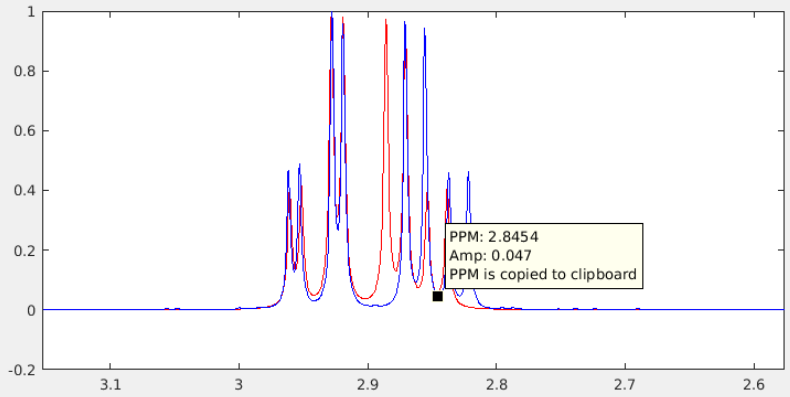
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04800

L-Asparagine(merged)

	10	11	12
10	2.8454	-16.1557	7.7280
11	-16.1557	2.9363	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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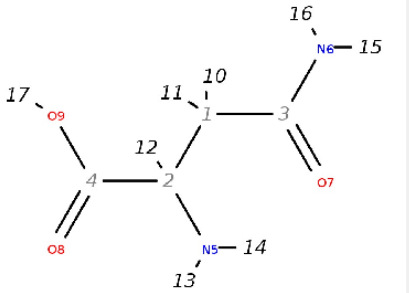
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:04

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

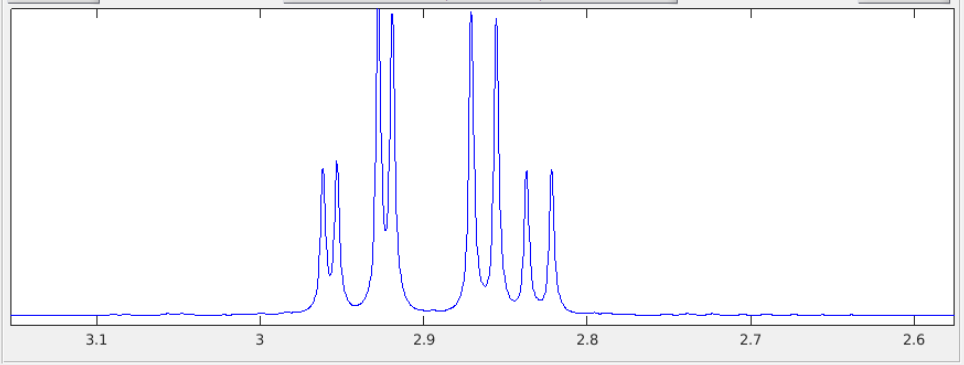
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

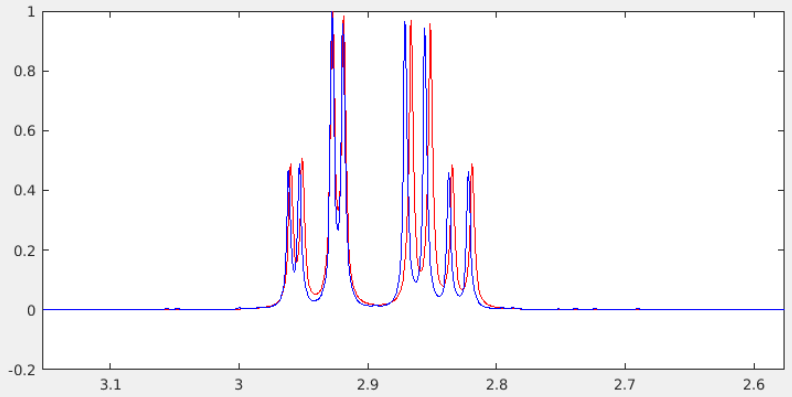
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.05603

L-Asparagine(merged)

	10	11	12
10	2.8454	-16.1557	7.7280
11	-16.1557	2.9363	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

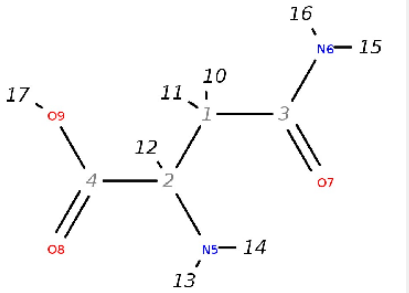
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:04

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1

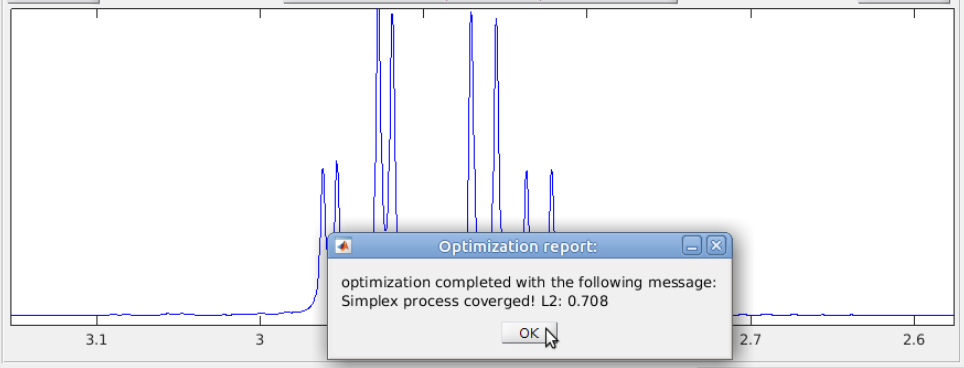


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 0.708

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

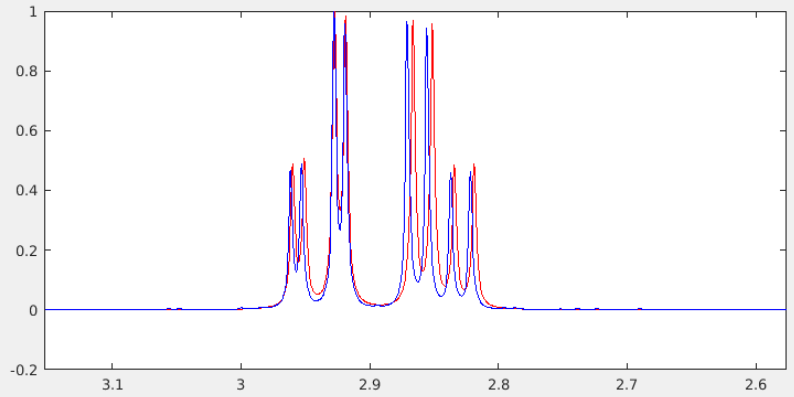
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.05603

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.7280
11	-16.9404	2.9371	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

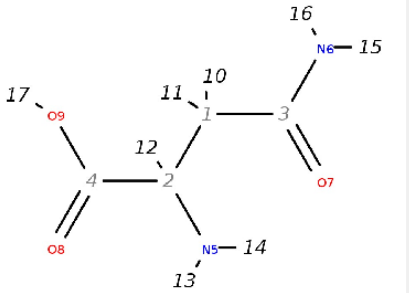
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:05

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

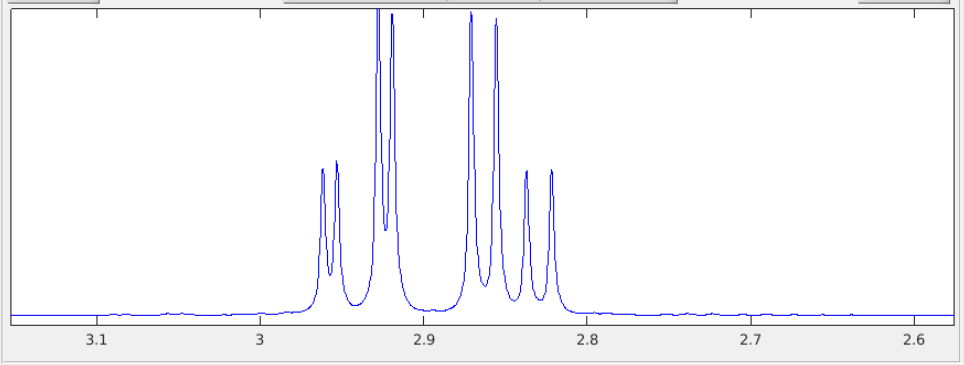
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

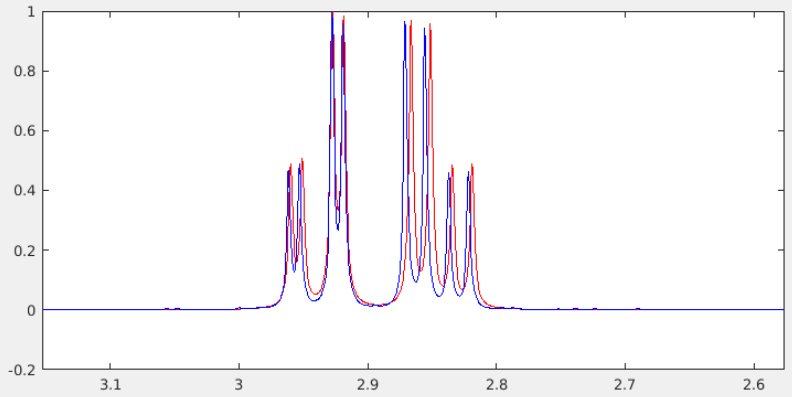
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.05603

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.7280
11	-16.9404	2.9371	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

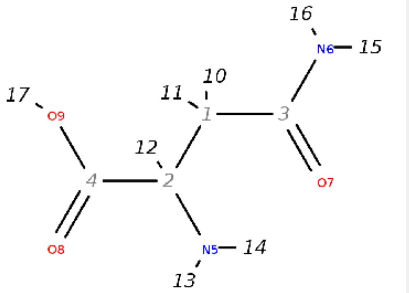
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:05

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

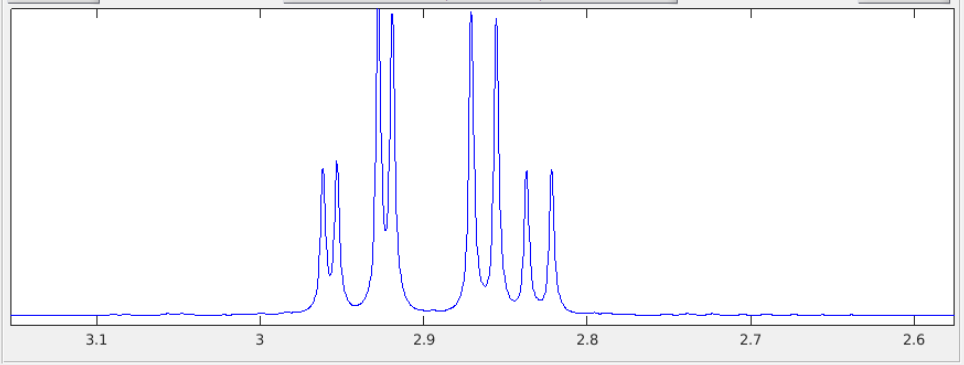
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

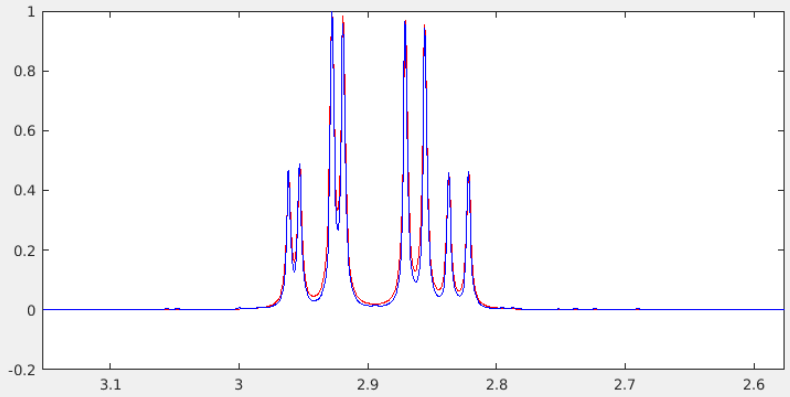
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01473

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.7280
11	-16.9404	2.9371	4.3600
12	7.7280	4.3600	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

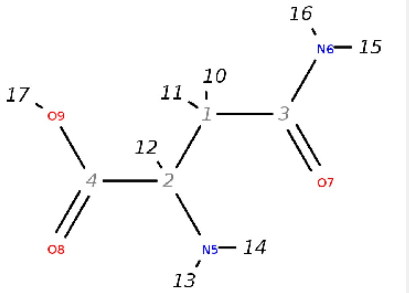
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:06

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

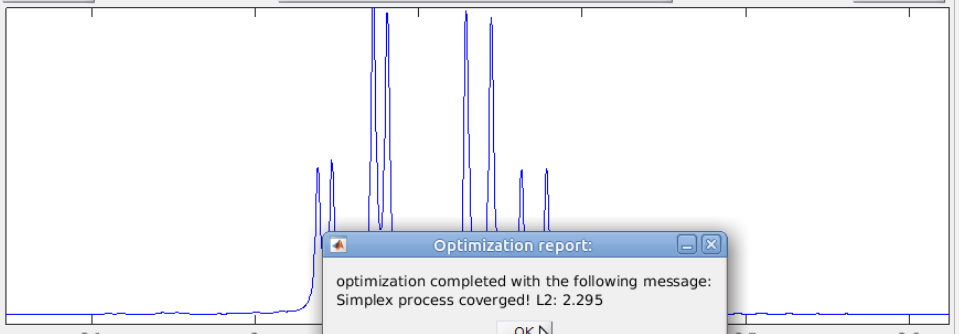
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 2.295

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

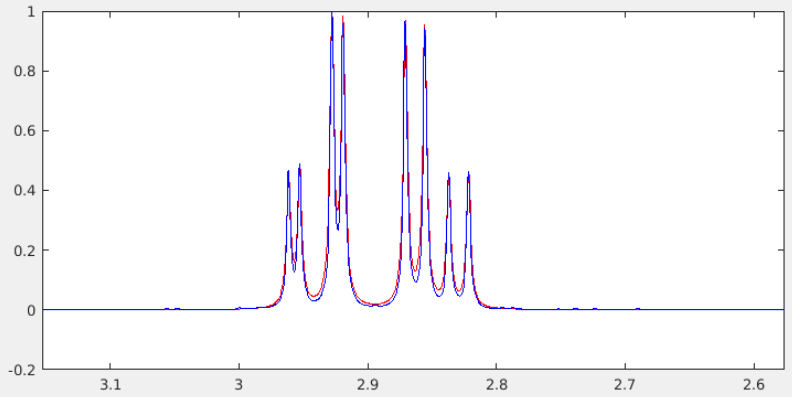
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01473

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

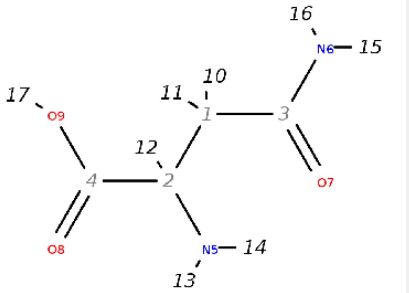
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:06

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

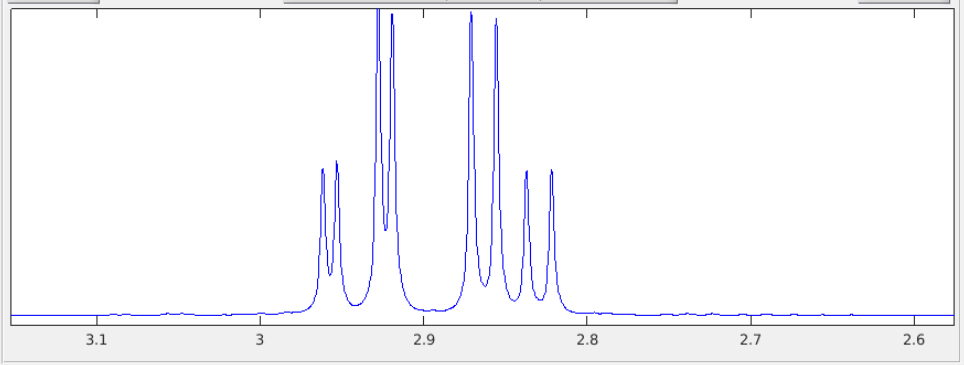
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

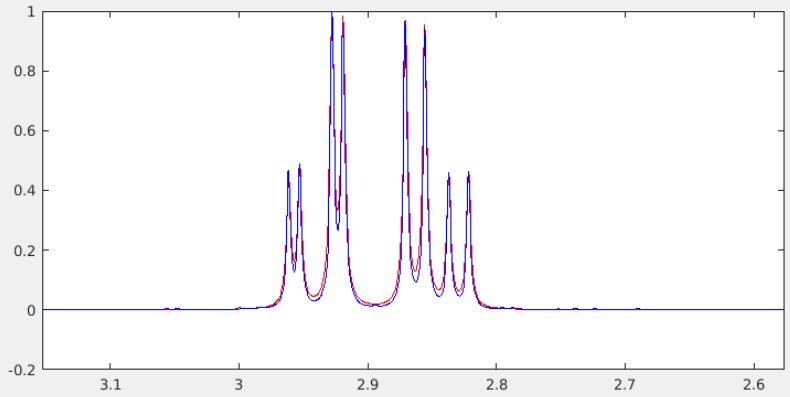
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01473

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

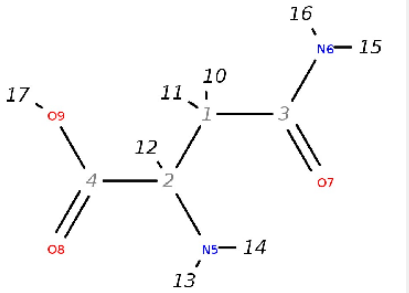
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:07

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

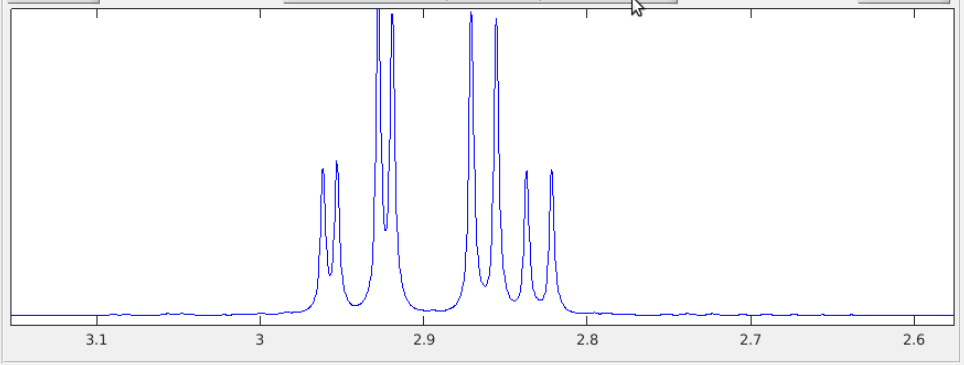
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

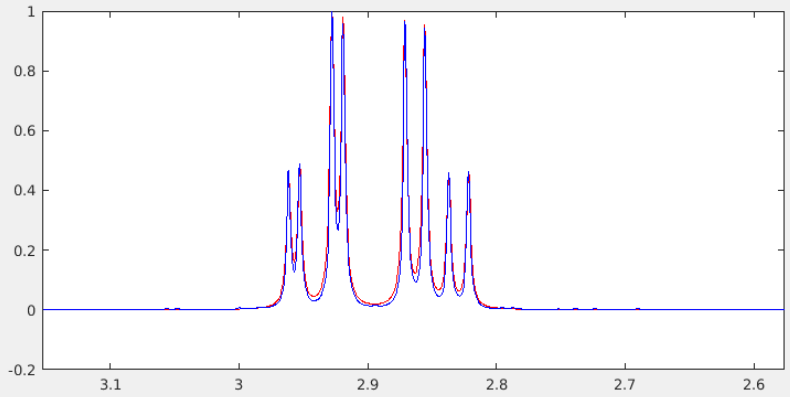
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

L-Asparagine(merged)

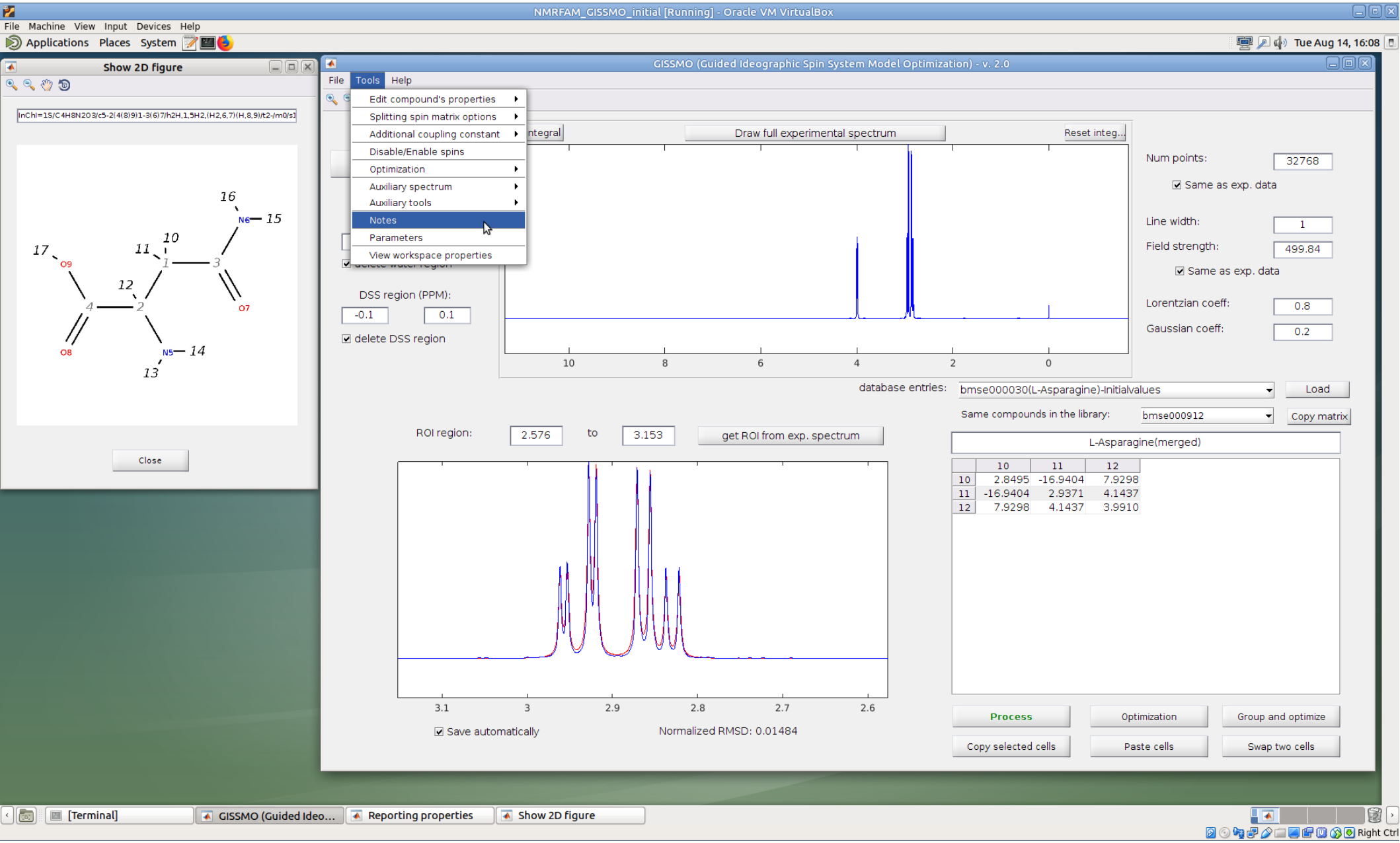
	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

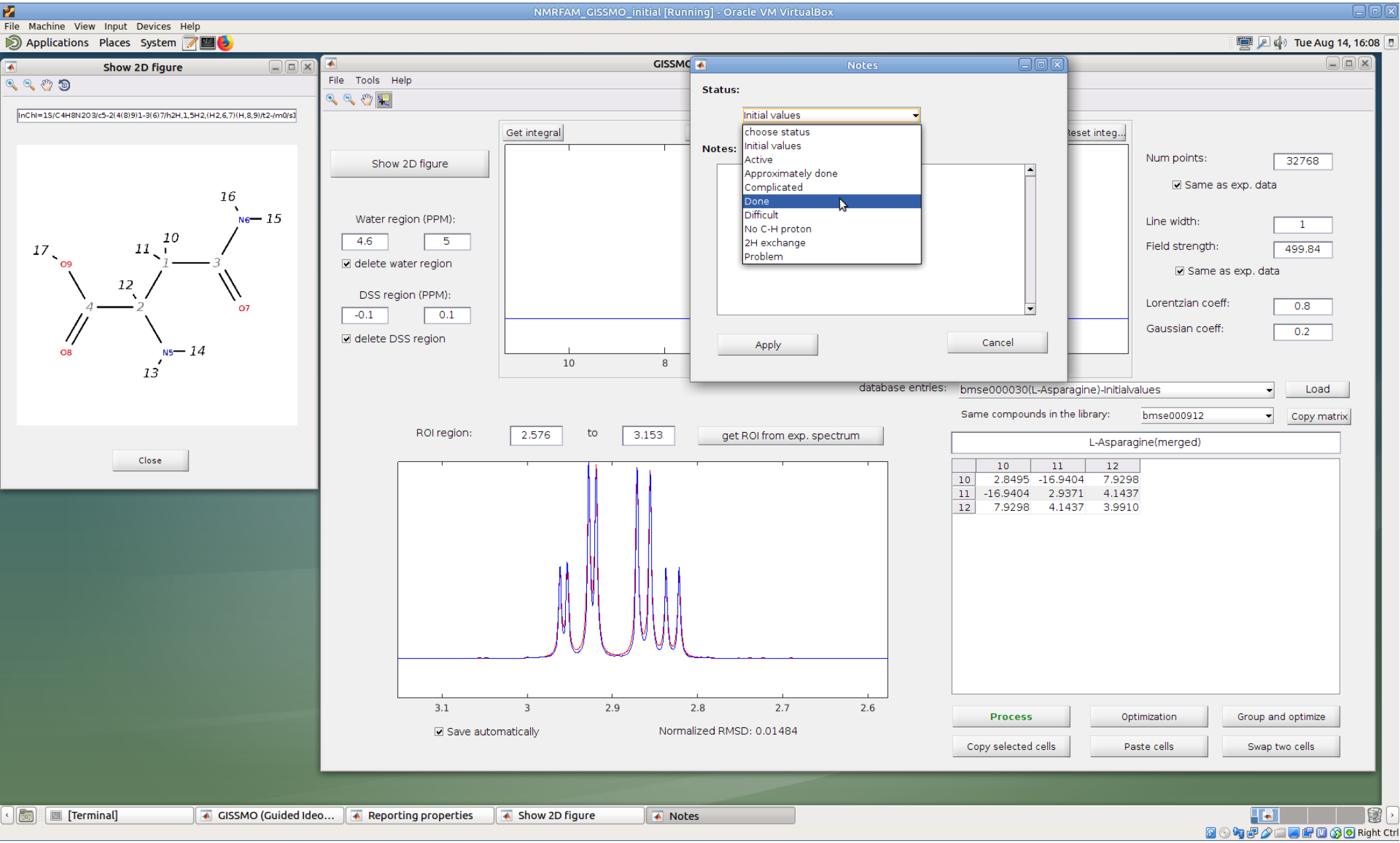
Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 16:08
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
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 integ...
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:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
2.576
to
3.153
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.8495 -16.9404 7.9298
11 -16.9404 2.9371 4.1437
12 7.9298 4.1437 3.9910
Save automatically
Normalized RMSD: 0.01484
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Tue Aug 14, 16:08
Show 2D figure
InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1
Close
GISSMO
File Tools Help
Notes
Status:
Initial values
choose status
Initial values
Active
Approximately done
Complicated
Done
Difficult
No C-H proton
2H exchange
Problem
Notes:
Apply
Cancel
Get integral
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000030(L-Asparagine)-Initialvalues
Load
Same compounds in the library:
bmse000912
Copy matrix
ROI region:
2.576
to
3.153
get ROI from exp. spectrum
L-Asparagine(merged)
10 11 12
10 2.8495 -16.9404 7.9298
11 -16.9404 2.9371 4.1437
12 7.9298 4.1437 3.9910
Save automatically
Normalized RMSD: 0.01484
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Notes
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

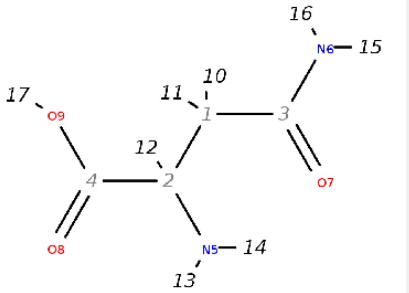
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:09

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

GISSMO

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

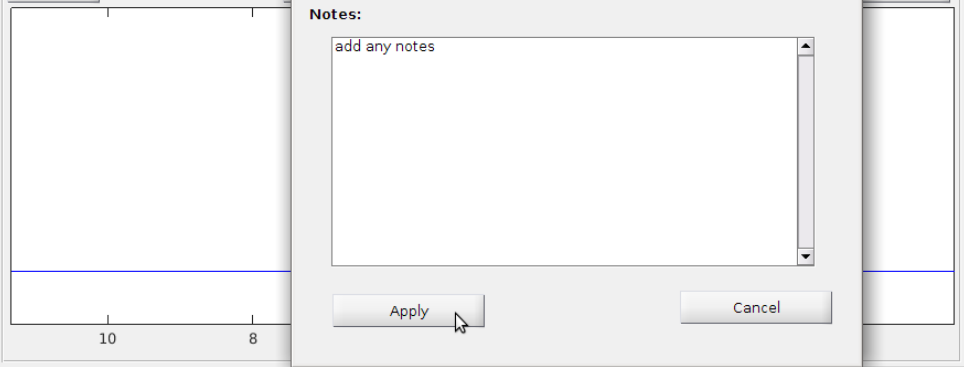
DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset integ...



Notes

Status:

Done

Notes:

add any notes

Apply

Cancel

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

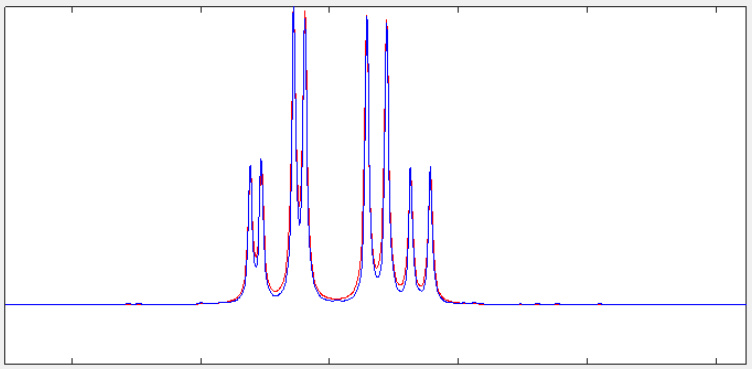
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 2.576 to 3.153 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

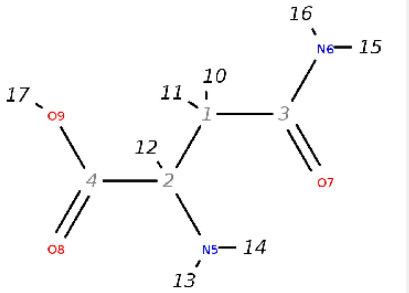
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:09

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

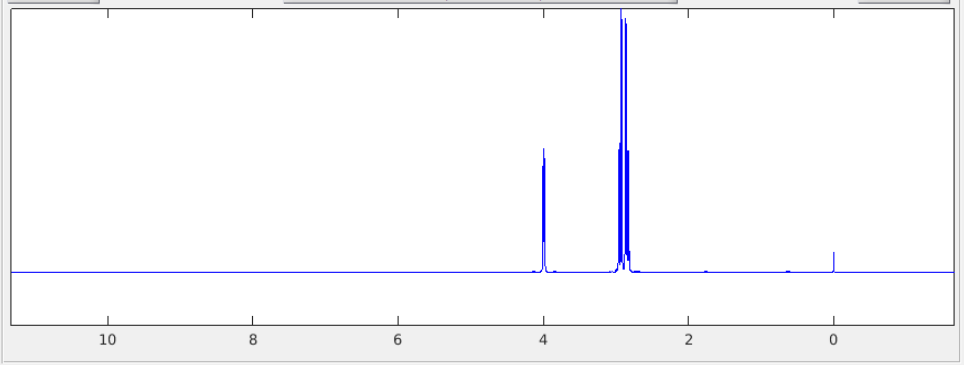
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

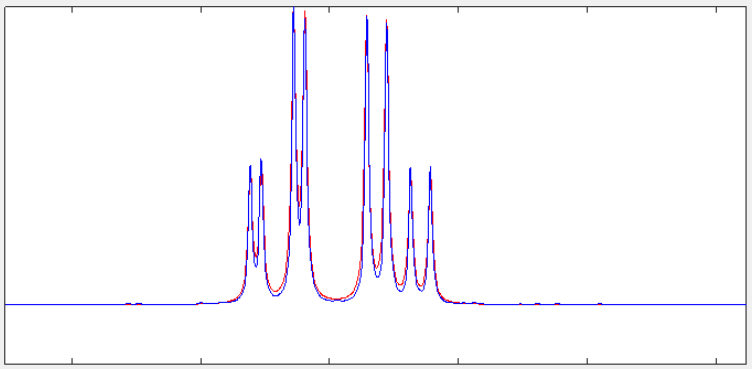
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000030(L-Asparagine)-Done | Load | Copy matrix

bmse000025(D-(+)-Threo-isocitricacid)-Initialvalues
bmse000026(D-(+)-Xylose)-Initialvalues
bmse000027(D-Xylulose)-Initialvalues
bmse000028(L-Alanine)-Initialvalues
bmse000029(L-Arginine)-Initialvalues
bmse000030(L-Asparagine)-Done
bmse000031(L-Asparticacid)-Initialvalues
bmse000032(L-Citrulline)-Initialvalues
bmse000033(L-Cystathionine)-Initialvalues
bmse000034(L-Cysteine)-Initialvalues
bmse000035(L-Cystine)-Initialvalues
bmse000036(L-(-)-Fucose)-Initialvalues
bmse000037(L-Glutamicacid)-Initialvalues
bmse000038(L-Glutamine)-Initialvalues
bmse000039(L-Histidine)-Initialvalues
bmse000040(L-Homoserine)-Initialvalues
bmse000041(L-Isoleucine)-Initialvalues
bmse000042(L-Leucine)-Initialvalues
bmse000043(L-Lysine)-Initialvalues
bmse000044(L-Methionine)-Initialvalues

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

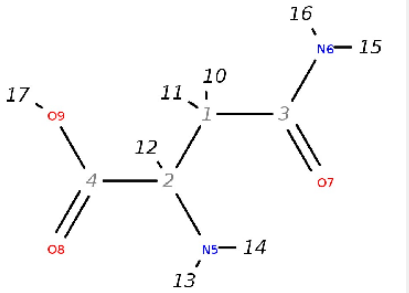
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:10

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

Show 2D figure

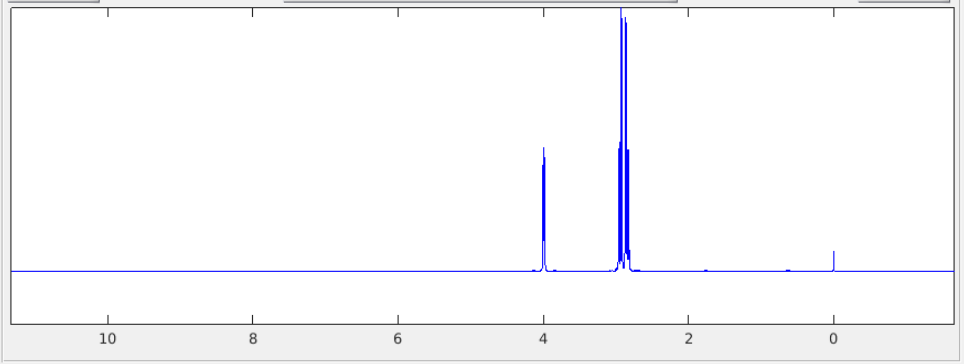
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

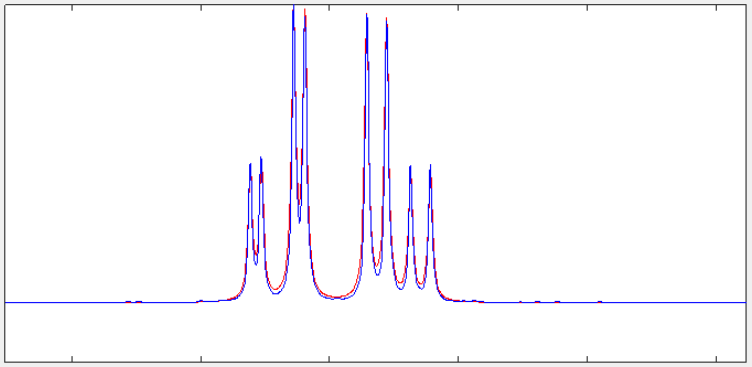
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000031(L-Asparticacid)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

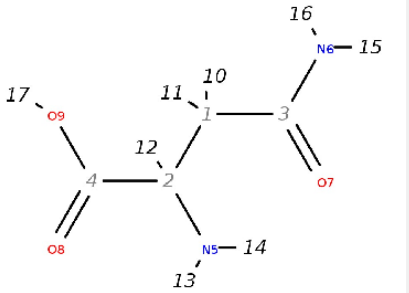
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:10

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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

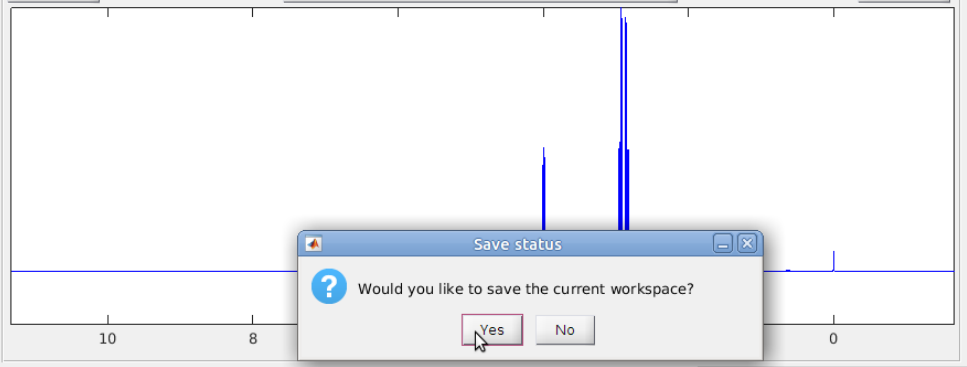
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Save status

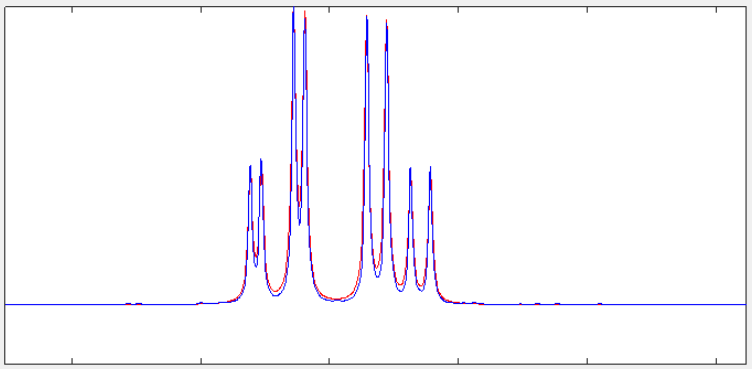
Would you like to save the current workspace?

Yes No

database entries: bmse000031(L-Asparticacid)-Initialvalues Load

Same compounds in the library: bmse000912 Copy matrix

ROI region: 2.576 to 3.153 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

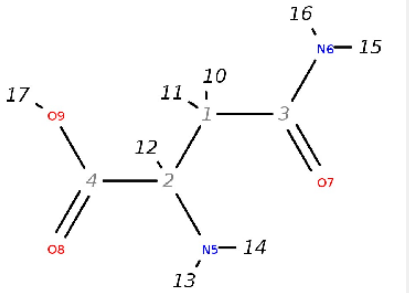
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:10

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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

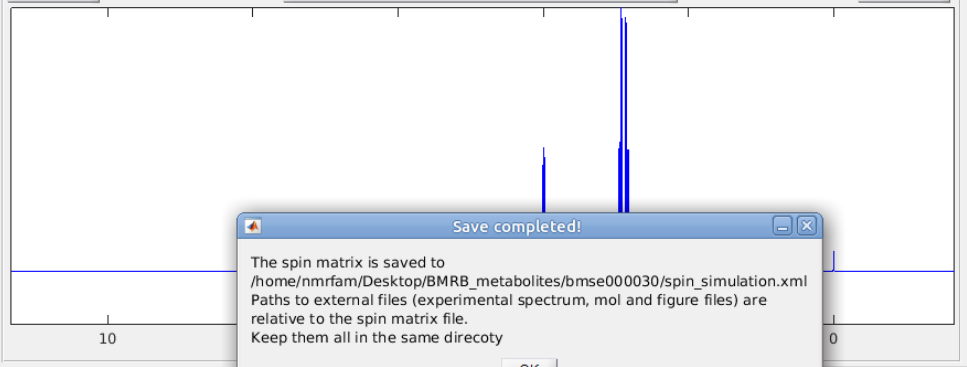
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Save completed!

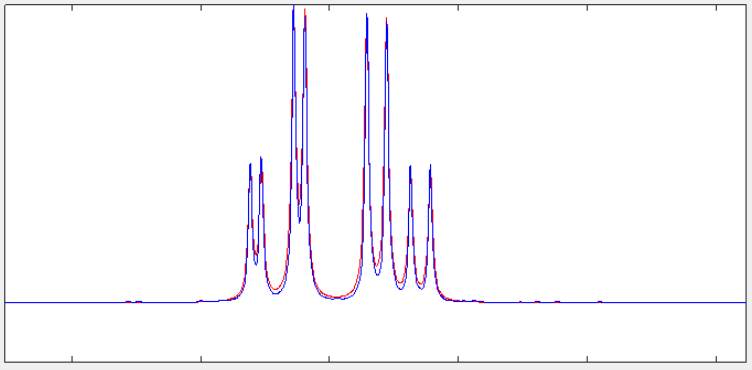
The spin matrix is saved to
/home/nmrfam/Desktop/BMRB_metabolites/bmse000030/spin_simulation.xml
Paths to external files (experimental spectrum, mol and figure files) are relative to the spin matrix file.
Keep them all in the same direcoty

OK

Asparticacid)-Initialvalues | Load

Same compounds in the library: bmse000912 | Copy matrix

ROI region: 2.576 to 3.153 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01484

L-Asparagine(merged)

	10	11	12
10	2.8495	-16.9404	7.9298
11	-16.9404	2.9371	4.1437
12	7.9298	4.1437	3.9910

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

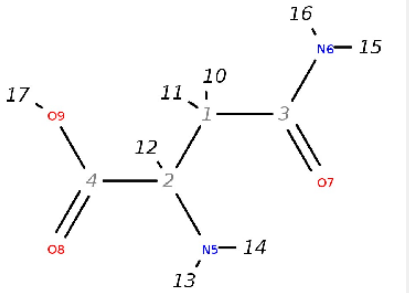
File Machine View Input Devices Help

Applications Places System

Tue Aug 14, 16:11

Show 2D figure

InChI=1S/C4H8N2O3/c5-2(4(8)9)1-3(6)7/h2H,1,5H2,(H2,6,7)(H,8,9)/t2-/m0/s1



Close

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

File Tools Help

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

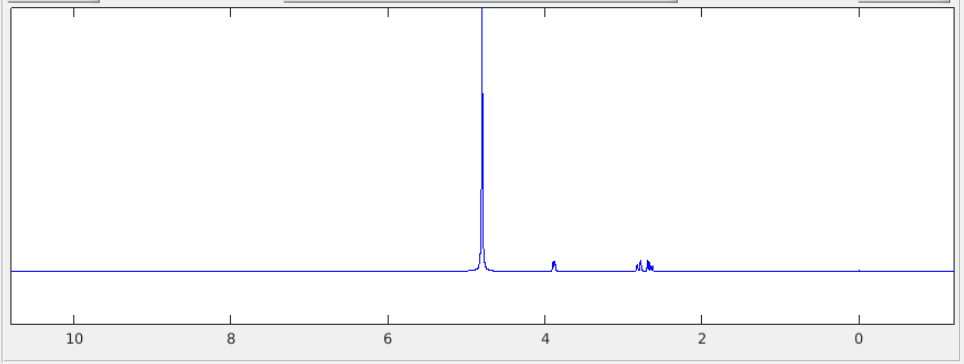
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 400.13

Same as exp. data

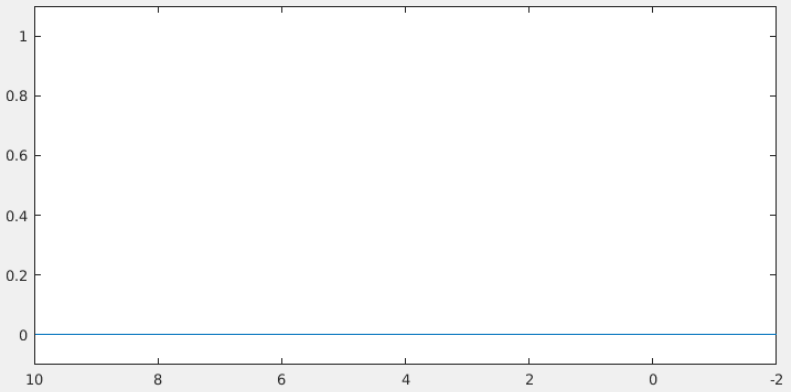
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000031(L-Asparticacid)-Initialvalues | Load

Same compounds in the library: bmse000273 | Copy matrix

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



Save automatically

simulation info

L-Aspartic acid(merged)

	10	11	12
10	2.6497	-12.4000	9.1100
11	-12.4000	2.7150	9.1100
12	9.1100	9.1100	4.3253

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl