

nmrfam's Home

BMRB\_metabolites

GISSMO\_v2

Maybridge\_RO3\_library

milo on brown

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

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

simulation info

☒ Save automatically

Get integral Draw full experimental spectrum Reset integral

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:

bmse000537(2-methylnaphthalene)-Initialvalues

bmse000762(neostigmine)-Initialvalues

bmse000763(nonactin)-Initialvalues

bmse000764(Nonadecane)-Initialvalues

bmse000765(octamethylcyclotetrasiloxane)-Initialvalues

bmse000766(orthanilicacid)-Initialvalues

bmse000767(Propionicacid)-Initialvalues

bmse000768(saligenin)-Initialvalues

bmse000769(alpha-Lipoamide)-Initialvalues

bmse000770(Phenylbeta-D-glucoside)-Initialvalues

bmse000771(Pyromelliticacid)-Initialvalues

bmse000772(SalicylhydroxamicAcid)-Initialvalues

bmse000773(triethylenetetramine)-Initialvalues

bmse000774(TrimethylPhosphate)-Initialvalues

bmse000775(3-Methoxybenzamide)-Initialvalues

bmse000776(L-Anserine)-Initialvalues

bmse000777(TributylPhosphate)-Initialvalues

bmse000778(gamma-terpinene)-Initialvalues

bmse000779(Metoclopramide)-Initialvalues

bmse000780(Tetramethylammonium)-Initialvalues

bmse000781(thioacetamide)-Initialvalues

Load

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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Field strength: 400.13  
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Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000774(TrimethylPhosphate)-Initialvalues Load

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

simulation info

Save automatically

2-methylnaphthalene(merged)

	12	13	14	15	16	17	18	19
12	2.5003	0	0	0	0	0	0	1.3300
13	0	2.5003	-12.4000	0	0	0	0	1.3300
14	0	-12.4000	2.5003	0	0	0	0	1.3300
15	0	0	0	7.4785	6.8900	8.1300	1.3300	0.5000
16	0	0	0	6.8900	7.5633	1.3300	8	0.5000
17	0	0	0	8.1300	1.3300	8.0226	0.5000	0.5000
18	0	0	0	1.3300	8	0.5000	7.6762	0.5000
19	1.3300	1.3300	1.3300	0	0	0.5000	0	7.2950
20	0	0	0	0.5000	0	1.3300	0.5000	8.4300
21	1.3300	1.3300	1.3300	0	0.5000	0.5000	1.3300	1.3300

Process Optimization Group and optimize

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get ROI from exp. spectrum

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Gaussian coeff: 0.2

database entries: bmse000774(TrimethylPhosphate)-Initialvalues

Load

2-methylnaphthalene(merged)

	12	13	14	15	16	17	18	19
12	2.5003	0	0	0	0	0	0	1.3300
13	0	2.5003	-12.4000	0	0	0	0	1.3300
14	0	-12.4000	2.5003	0	0	0	0	1.3300
15	0	0	0	7.4785	6.8900	8.1300	1.3300	0.5000
16	0	0	0	6.8900	7.5633	1.3300	8	0.5000
17	0	0	0	8.1300	1.3300	8.0226	0.5000	0.5000
18	0	0	0	1.3300	8	0.5000	7.6762	0.5000
19	1.3300	1.3300	1.3300	0	0	0.5000	0	7.2950
20	0	0	0	0.5000	0	1.3300	0.5000	8.4300
21	1.3300	1.3300	1.3300	0	0.5000	0.5000	1.3300	1.3300

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4.6 5  
☒ delete water region

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

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

☒ Save automatically

simulation info

Trimethyl(Phosphate)-Initialvalues Load

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

2-methylnaphthalene(merged)

	12	13	14	15	16	17	18	19
12	2.5003	0	0	0	0	0	0	1.3300
13	0	2.5003	-12.4000	0	0	0	0	1.3300
14	0	-12.4000	2.5003	0	0	0	0	1.3300
15	0	0	0	7.4785	6.8900	8.1300	1.3300	0.5000
16	0	0	0	6.8900	7.5633	1.3300	8	0.5000
17	0	0	0	8.1300	1.3300	8.0226	0.5000	0.5000
18	0	0	0	1.3300	8	0.5000	7.6762	0.5000
19	1.3300	1.3300	1.3300	0	0	0.5000	0	7.2950
20	0	0	0	0.5000	0	1.3300	0.5000	8.4300
21	1.3300	1.3300	1.3300	0	0.5000	0.5000	1.3300	1.3300

Process Optimization Group and optimize

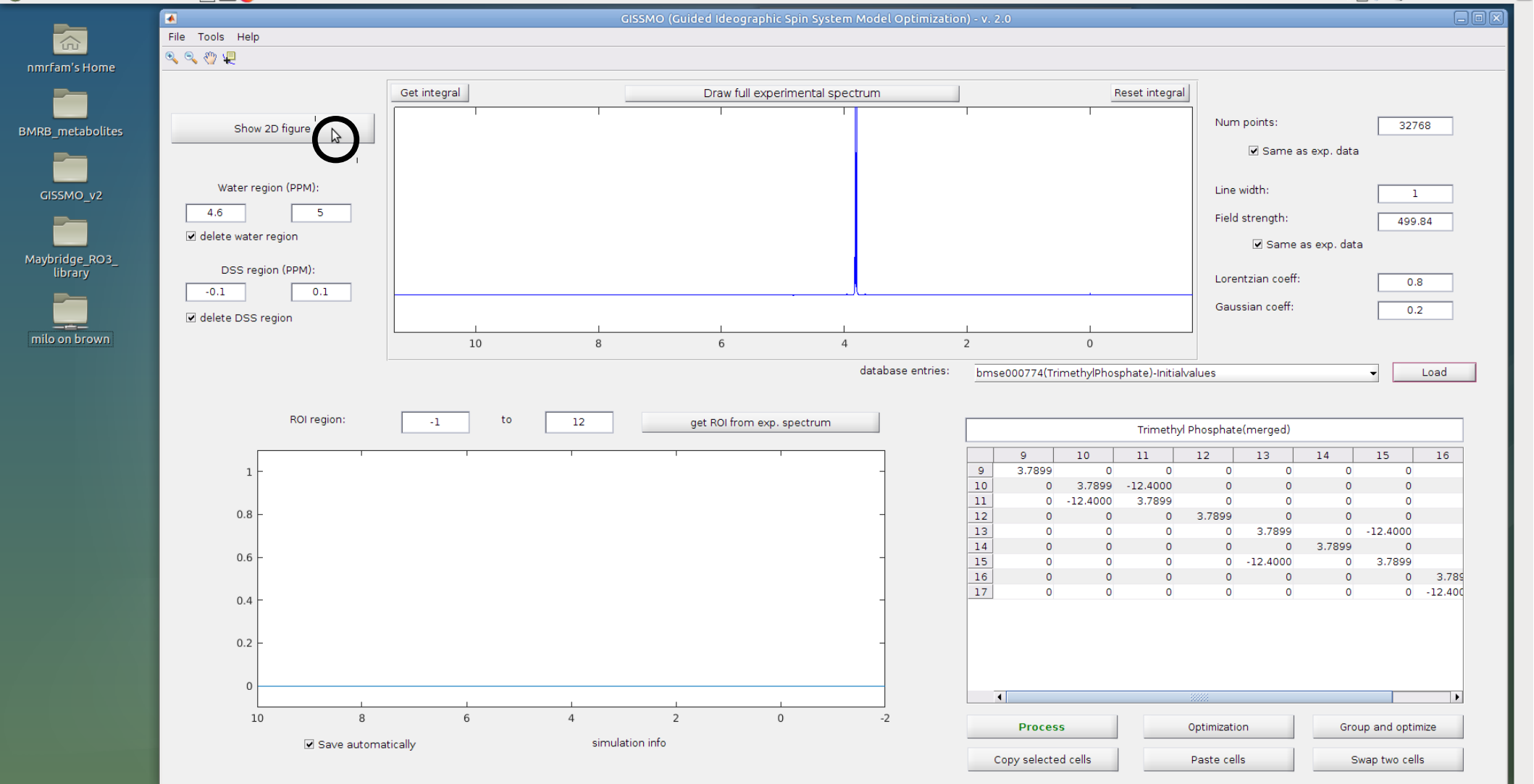
Copy selected cells Paste cells Swap two cells

Save completed!

The spin matrix is saved to  
/home/nmrfam/Desktop/BMRB\_metabolites/bmse000537/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 directory

OK





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GISSMO (Guided Ideogra

File Tools Help

Get integral

Draw full

Show 2D figure

Water region (PPM):

4.6 5

☒ delete water region

DSS region (PPM):

-0.1 0.1

☒ delete DSS region

ROI region: -1 to 12 get ROI from

1 0.8 0.6 0.4 0.2 0

10 8 6 4 2 0 -2

☒ Save automatically

simulation info

Should show 3-bond coupling to P

Show 2D figure

InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3

10 9 11 1 05 11 04 07 16 17 3 15 06 12 2 14 13

Close

32768

ne as exp. data

1

499.84

me as exp. data

eff: 0.8

ff: 0.2

Load

	14	15	16
0	0	0	0
0	0	0	0
0	0	0	0
0	0	0	0
9	0	-12.4000	0
0	3.7899	0	0
15	0	0	0
16	0	0	0
17	0	0	0

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

bmse000309 [GISSMO\_v2] [Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure

Right Ctrl

Smiles: InChI=1S/C3H9O4P/c1-5-8(4,6-2)/7-3/h1-3H3

Close

Get integral
Draw full experimental spectrum
Reset inte...

Show 2D figure

Water region (PPM):

☒ delete water region

DSS region (PPM):

☒ delete DSS region

Num points:

☒ Same as exp. data

Line width:

Field strength:

☒ Same as exp. data

Lorentzian coeff:

Gaussian coeff:

database entries: bmse000774(TrimethylPhosphate)-Initialvalues Load

ROI region:  to  get ROI from exp. spectrum

☒ Save automatically

simulation info

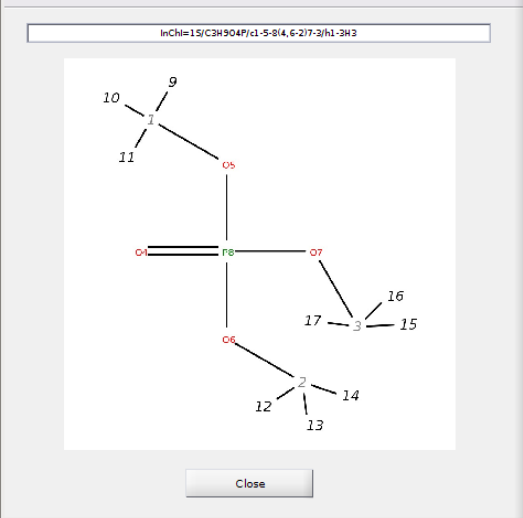
Trimethyl Phosphate(merged)							
	9	10	11	12	13	14	1
9	3.7899	0	0	0	0	0	0
10	0	3.7899	-12.4000	0	0	0	0
11	0	-12.4000	3.7899	0	0	0	0
12	0	0	0	3.7899	0	0	0
13	0	0	0	0	3.7899	0	-12.4000
14	0	0	0	0	0	3.7899	0
15	0	0	0	0	-12.4000	0	0
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0

Process
Optimization
Group and optimize

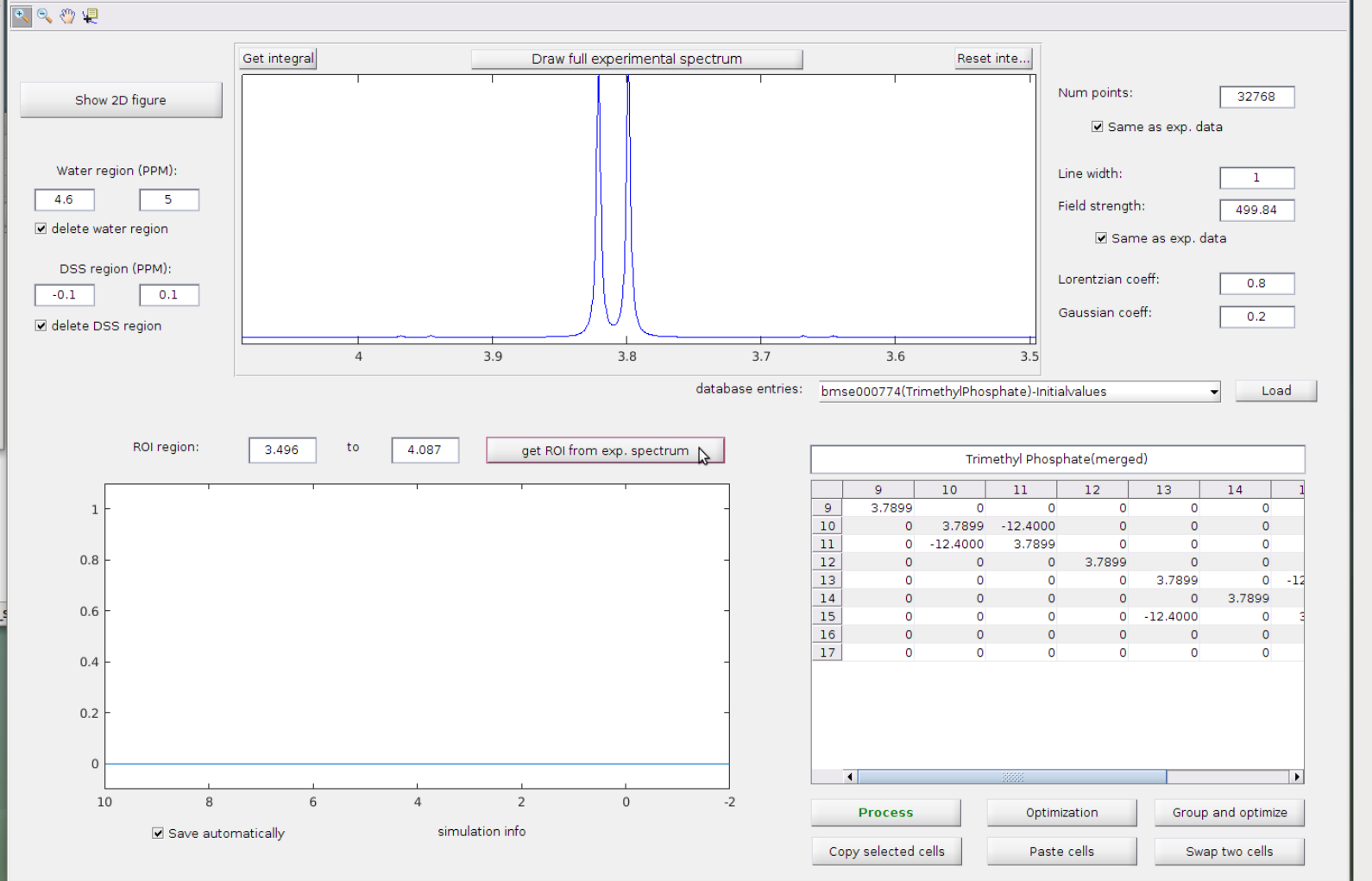
Copy selected cells
Paste cells
Swap two cells

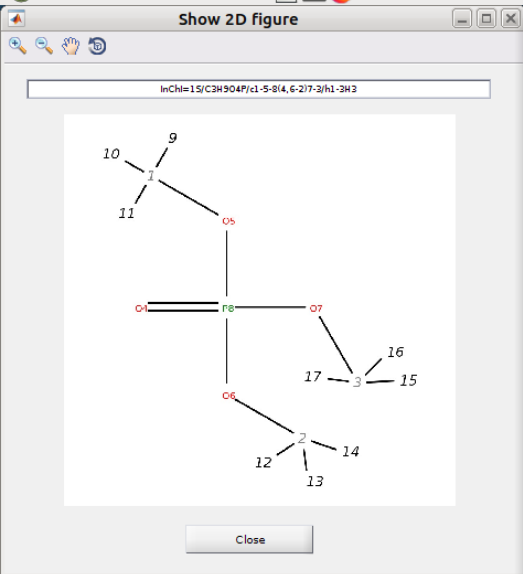
bmse000309 [GISSMO\_v2] [Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure

Right Ctrl

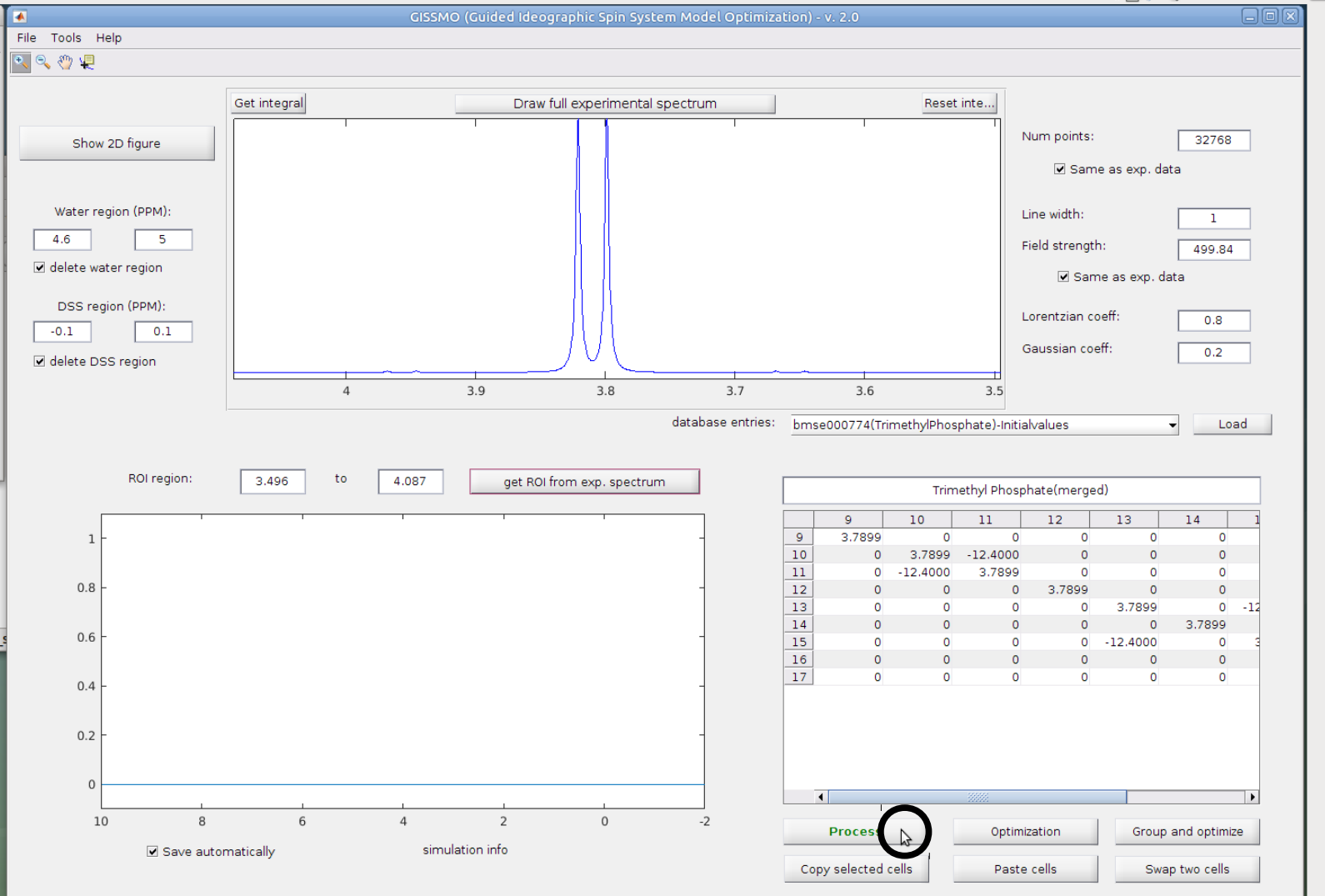


Network  
Brow...





Network  
Brow...



Show 2D figure

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

File Tools Help

Get integral Draw full experimental spectrum Reset inte...

Show 2D figure

Water region (PPM):

4.6 5

☒ delete water region

DSS region (PPM):

-0.1 0.1

☒ delete DSS region

database entries:

bmse000774(TrimethylPhosphate)-Initialvalues

Load

ROI region:

3.496 to 4.087

get ROI from exp. spectrum

☒ Save automatically

Normalized RMSD: 0.11228

Trimethyl Phosphate(merged)

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

9 10 11 12 13 14 15 16 17

3.7899 0 0 0 0 0 0 0 0

0 3.7899 -12.4000 0 0 0 0 0

0 -12.4000 3.7899 0 0 0 0 0

0 0 0 3.7899 0 0 0 0

0 0 0 0 3.7899 0 -12.4000 0

0 0 0 0 0 3.7899 0 0

0 0 0 0 0 0 -12.4000 0

0 0 0 0 0 0 0 3.7899

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0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

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9 10 11 12 13 14 15 16 17

3.7899 0 0 0 0 0 0 0 0

0 3.7899 -12.4000 0 0 0 0 0

0 -12.4000 3.7899 0 0 0 0 0

0 0 0 3.7899 0 0 0 0

0 0 0 0 3.7899 0 -12.4000 0

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0 0 0 0 0 0 -12.4000 0

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9 10 11 12 13 14 15 16 17

3.7899 0 0 0 0 0 0 0 0

0 3.7899 -12.4000 0 0 0 0 0

0 -12.4000 3.7899 0 0 0 0 0

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0 0 0 0 3.7899 0 -12.4000 0

0 0 0 0 0 3.7899 0 0

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0 0 0 0 0 0 0 0

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9 10 11 12 13 14 15 16 17

3.7899 0 0 0 0 0 0 0 0

0 3.7899 -12.4000 0 0 0 0 0

0 -12.4000 3.7899 0 0 0 0 0

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9 10 11 12 13 14 15 16 17

3.7899 0 0 0 0 0 0 0 0

0 3.7899 -12.4000 0 0 0 0 0

0 -12.4000 3.7899 0 0 0 0 0

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0 0 0 0 0 0 -12.4000 0

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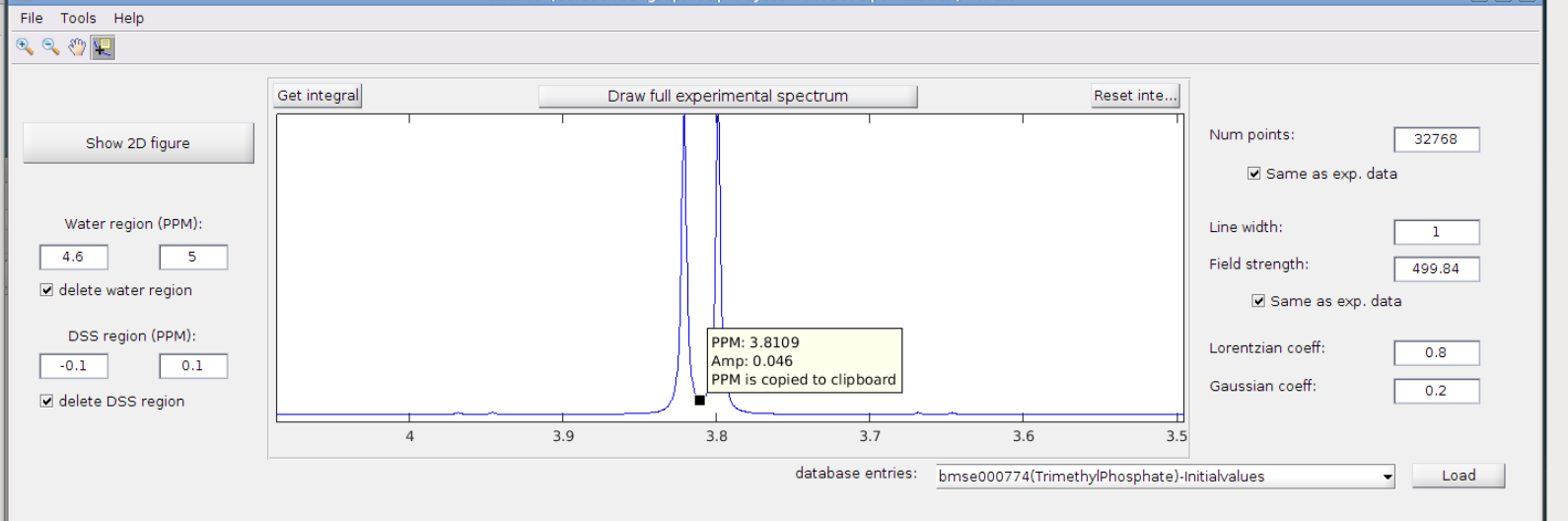
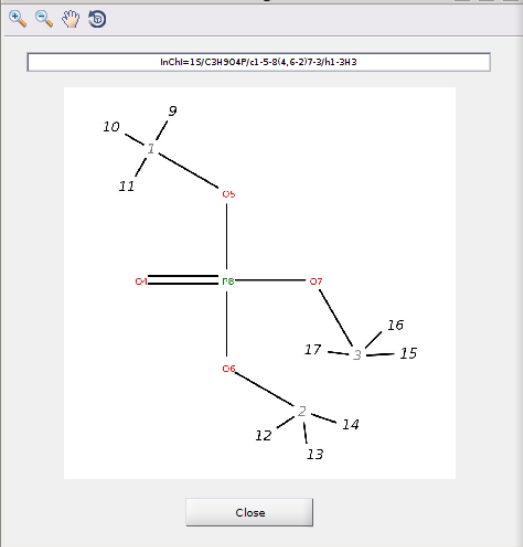
0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

0 0 0 0 0 0 0 0

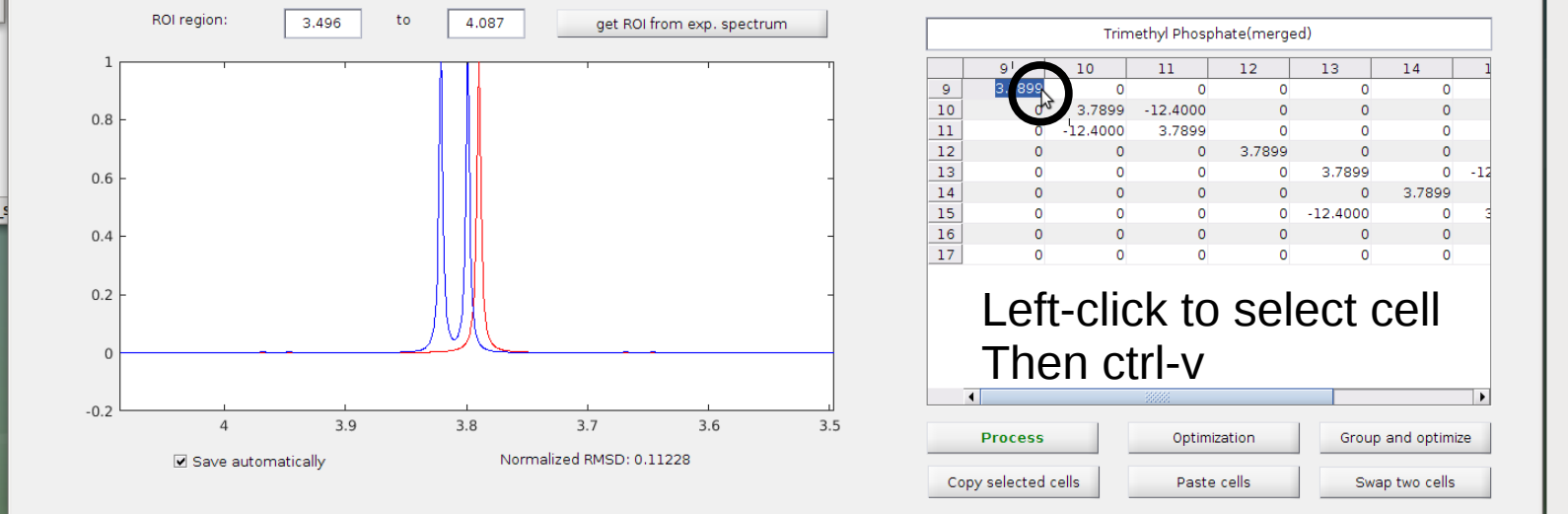
0 0 0 0 0 0 0

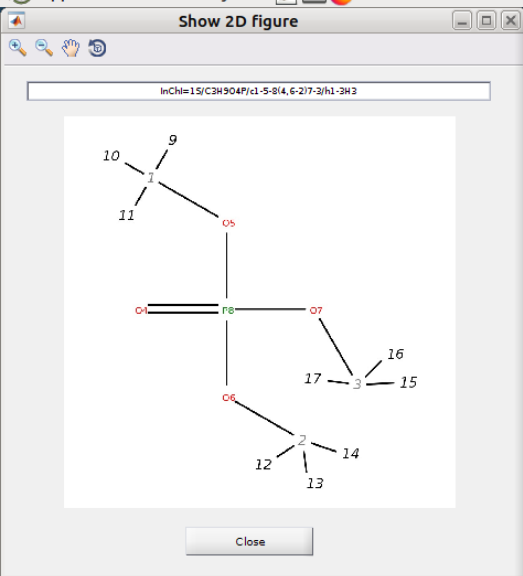


Network

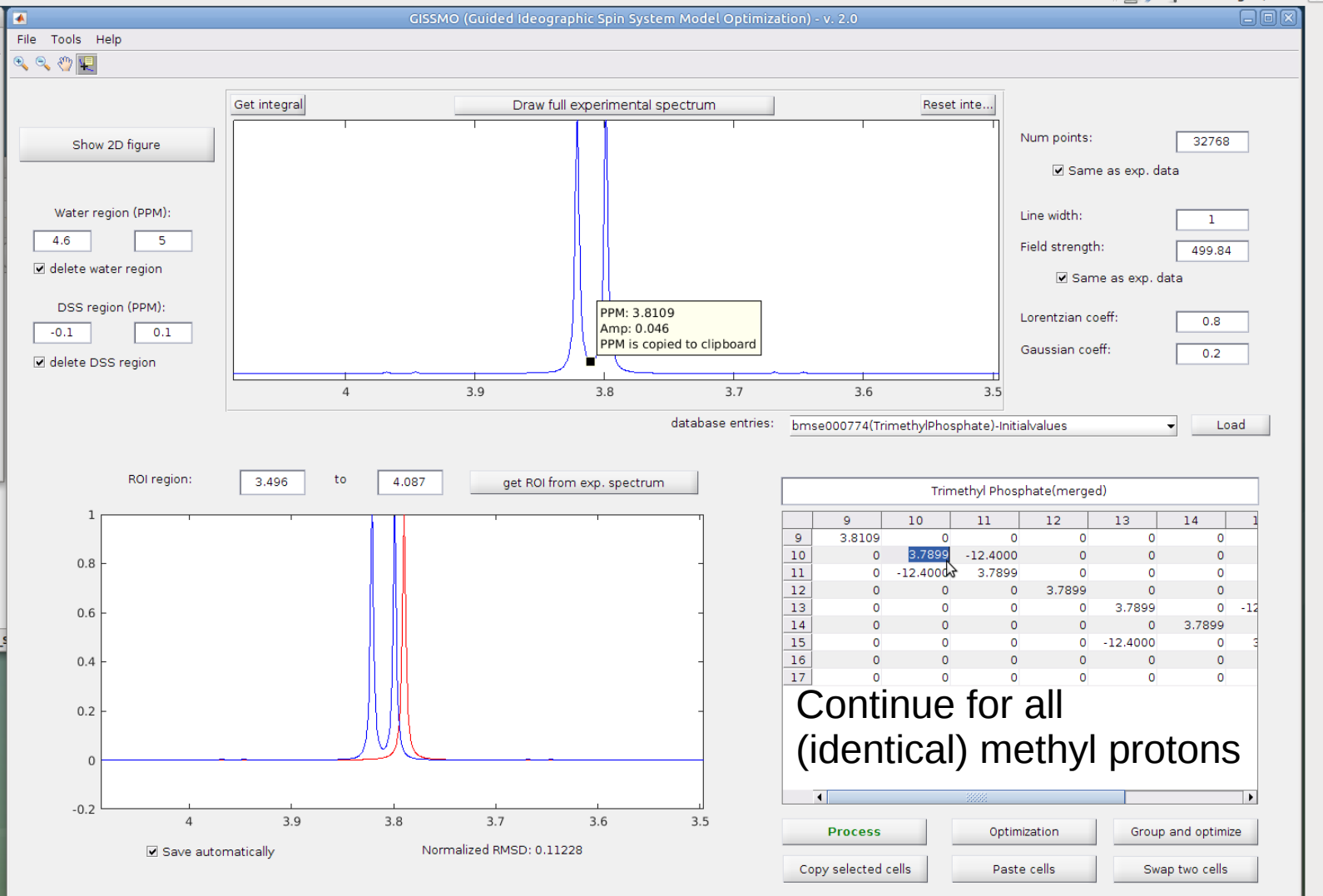
Brow...

\*spin\_s

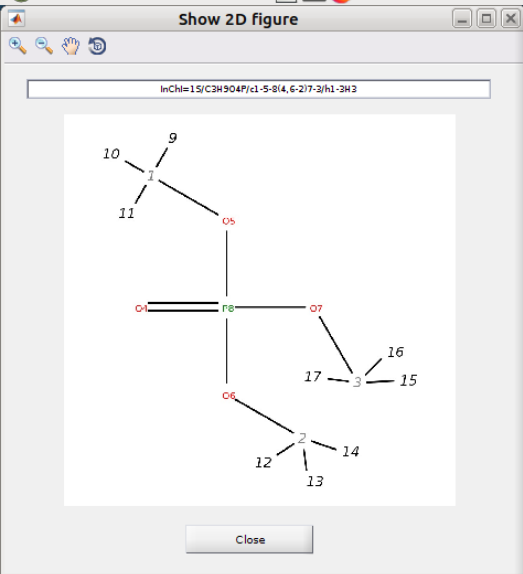




Network  
Brow...



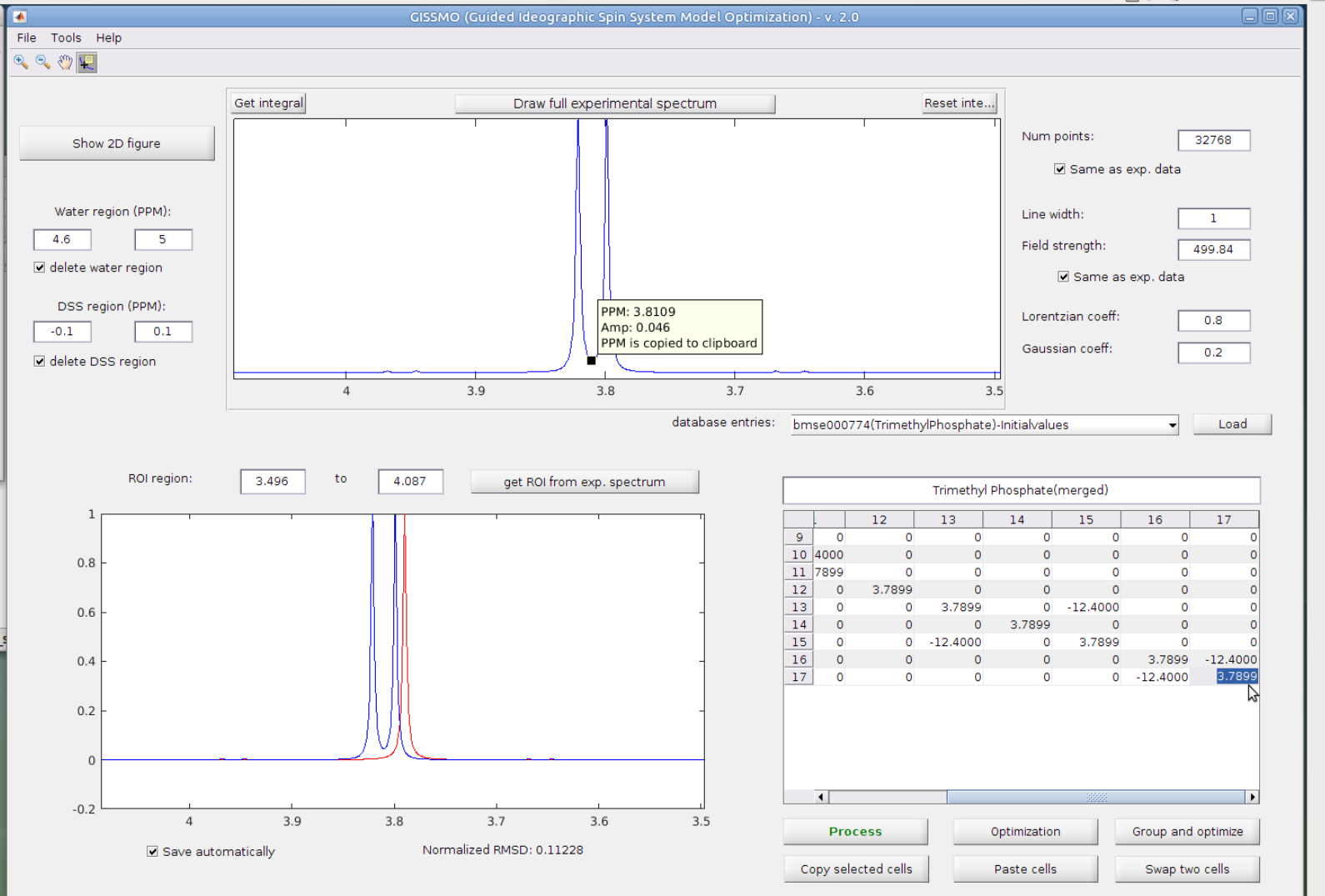


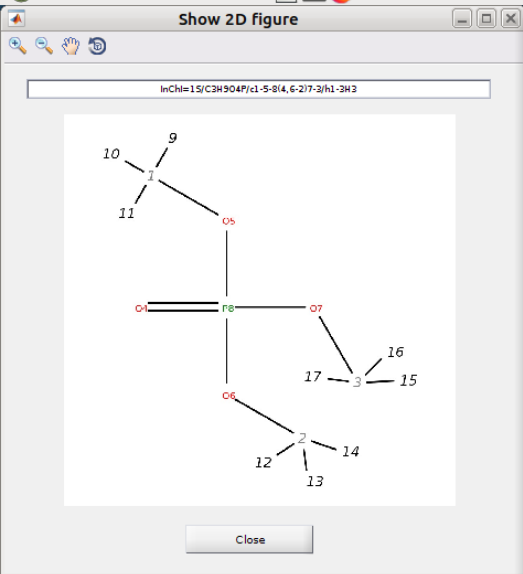


Network

Brow...

\*spin\_s

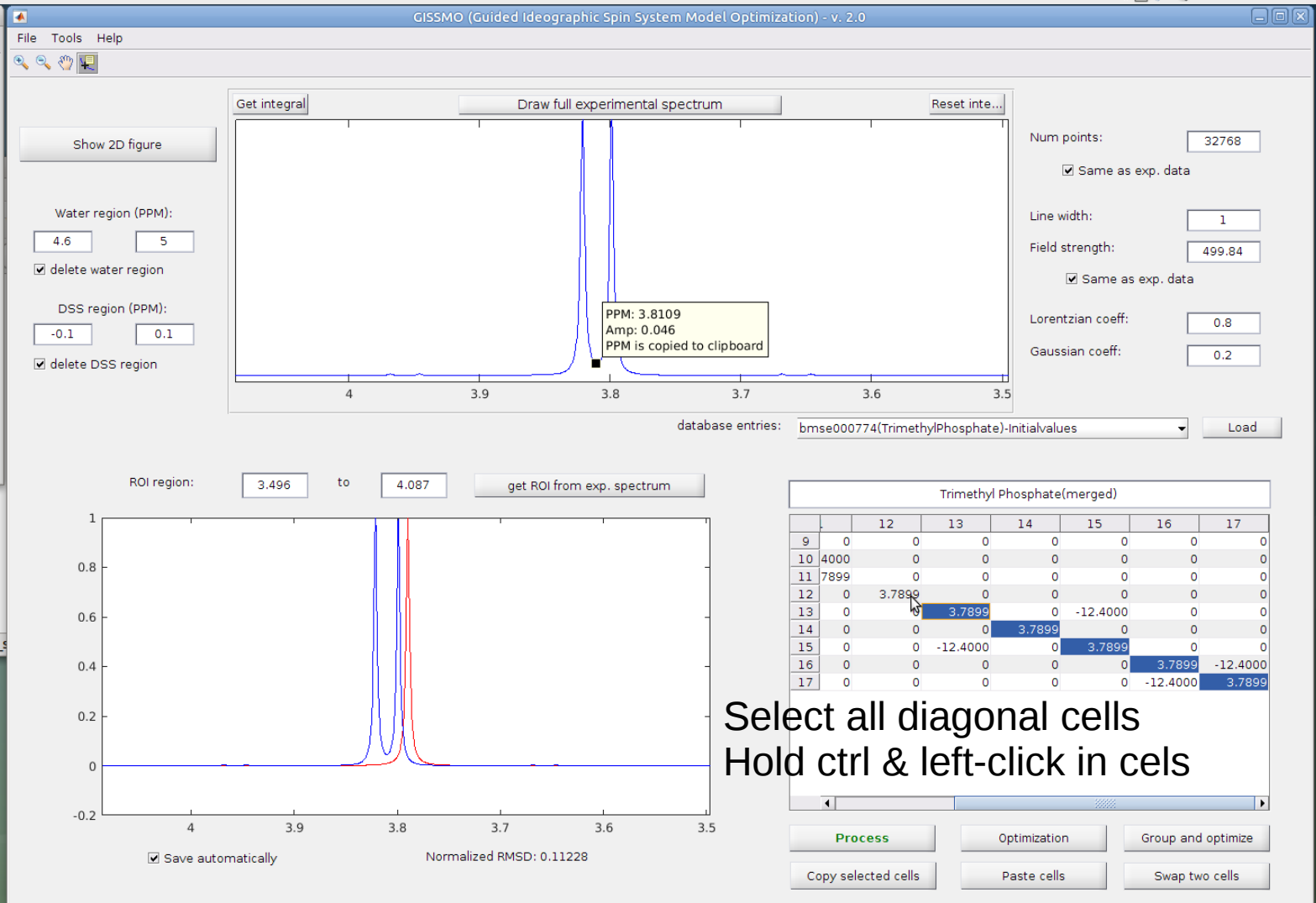


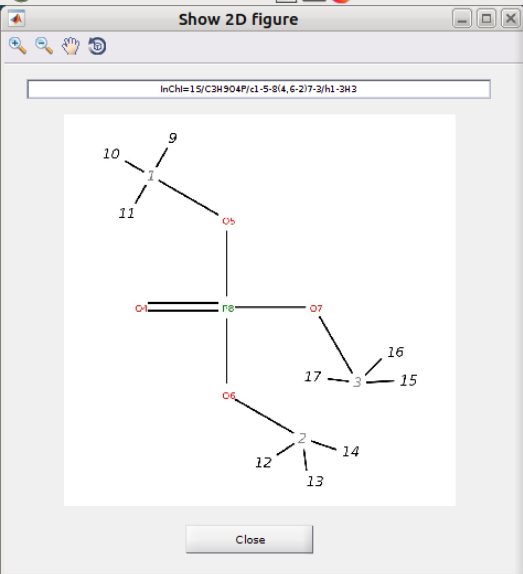


Network

Brow...

\*spin\_s

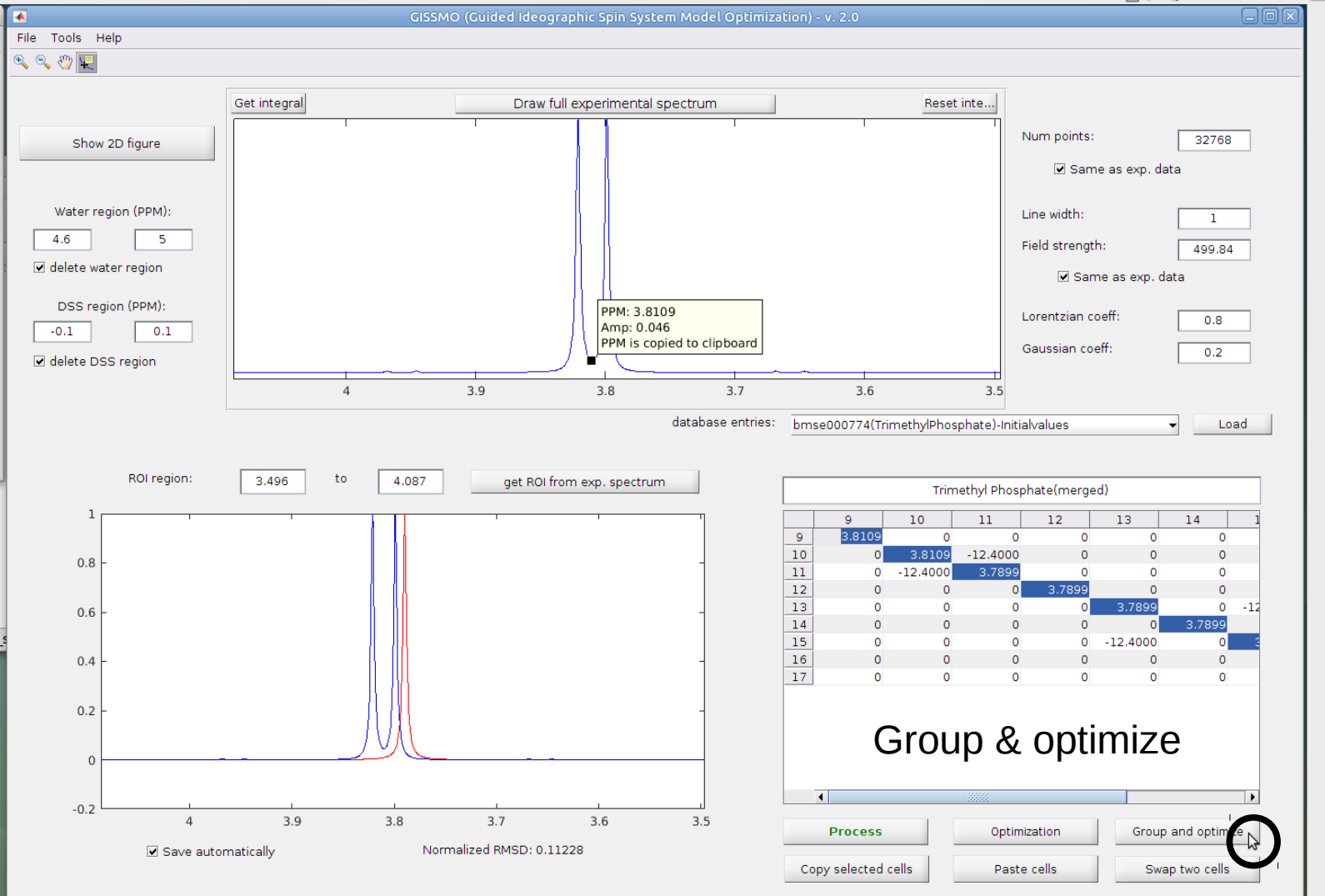


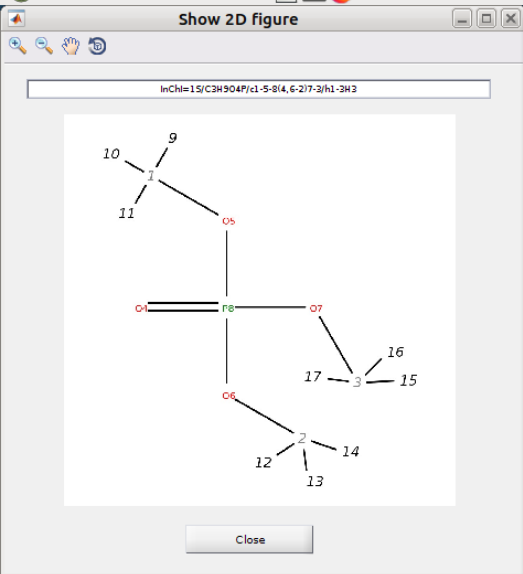


Network

Brow...

\*spin\_s

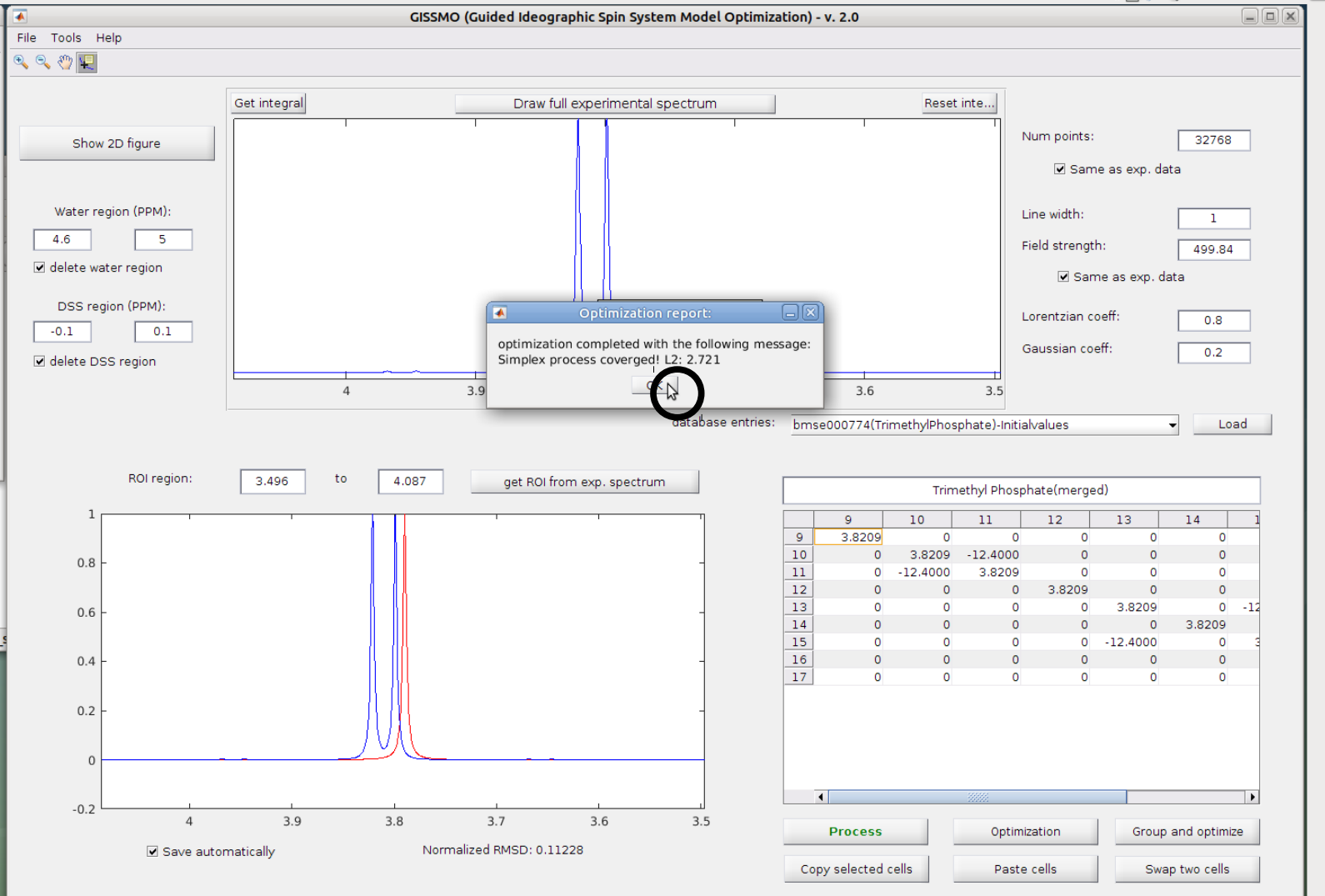


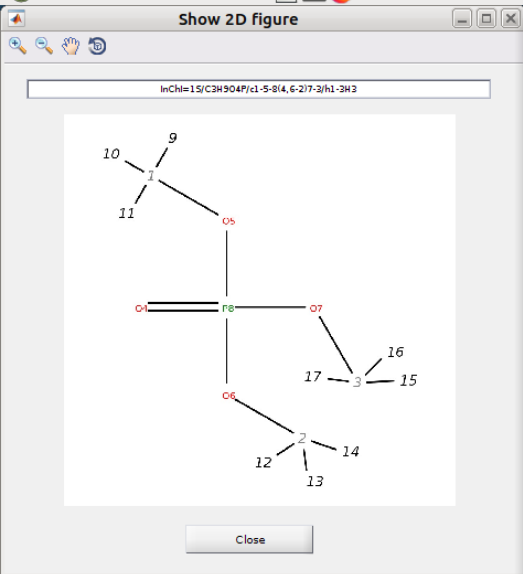


Network

Brow...

\*spin\_s

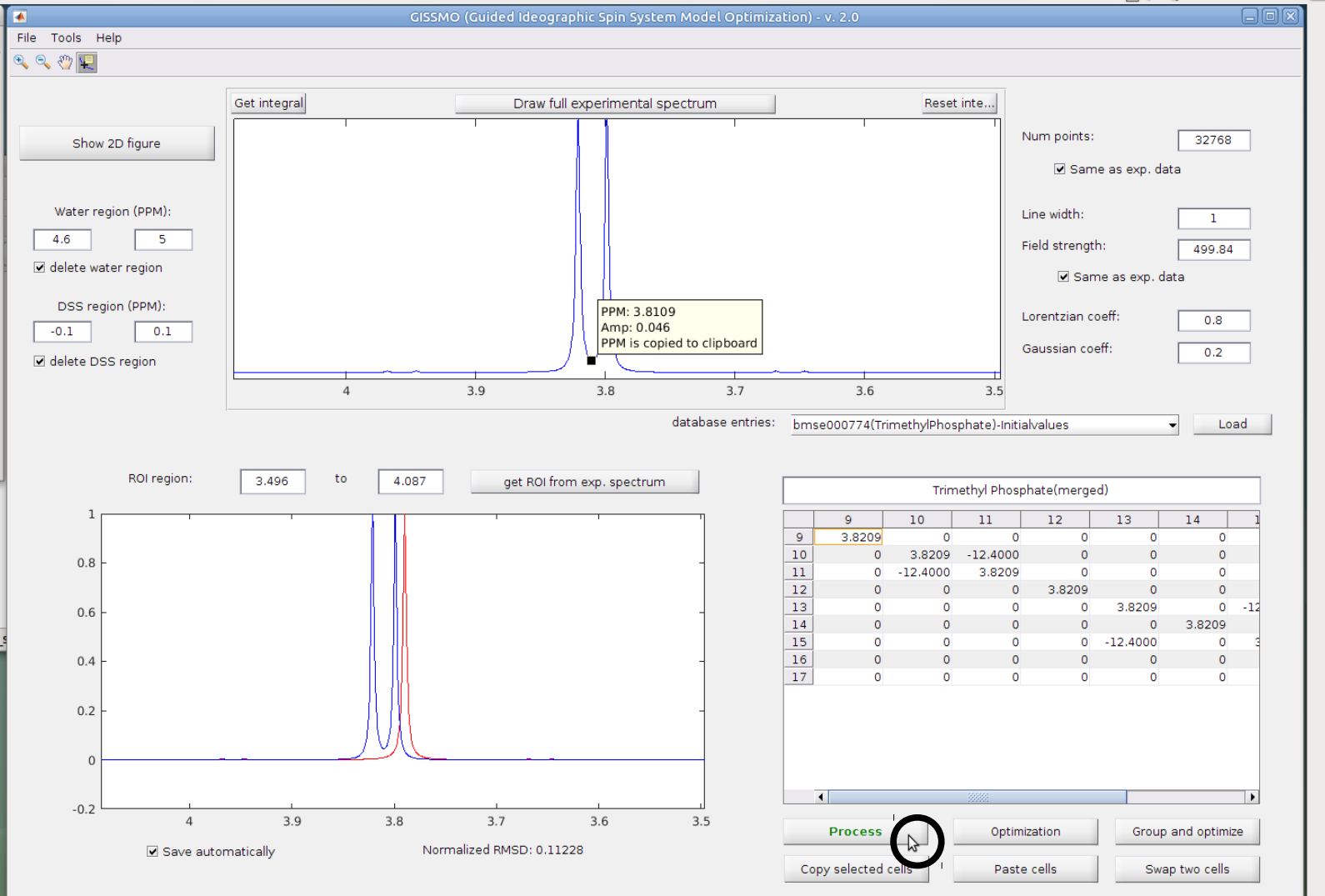


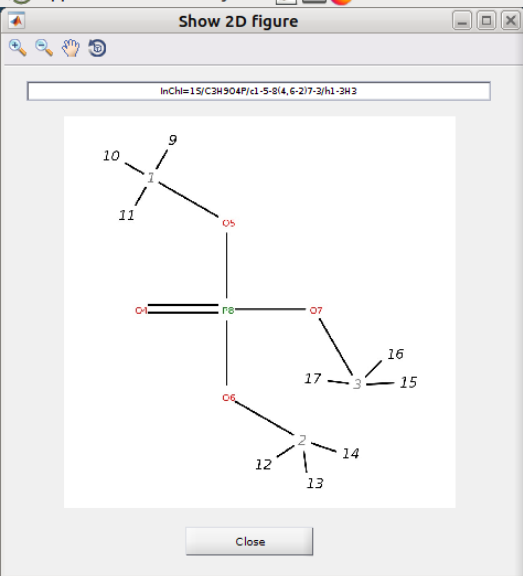


Network

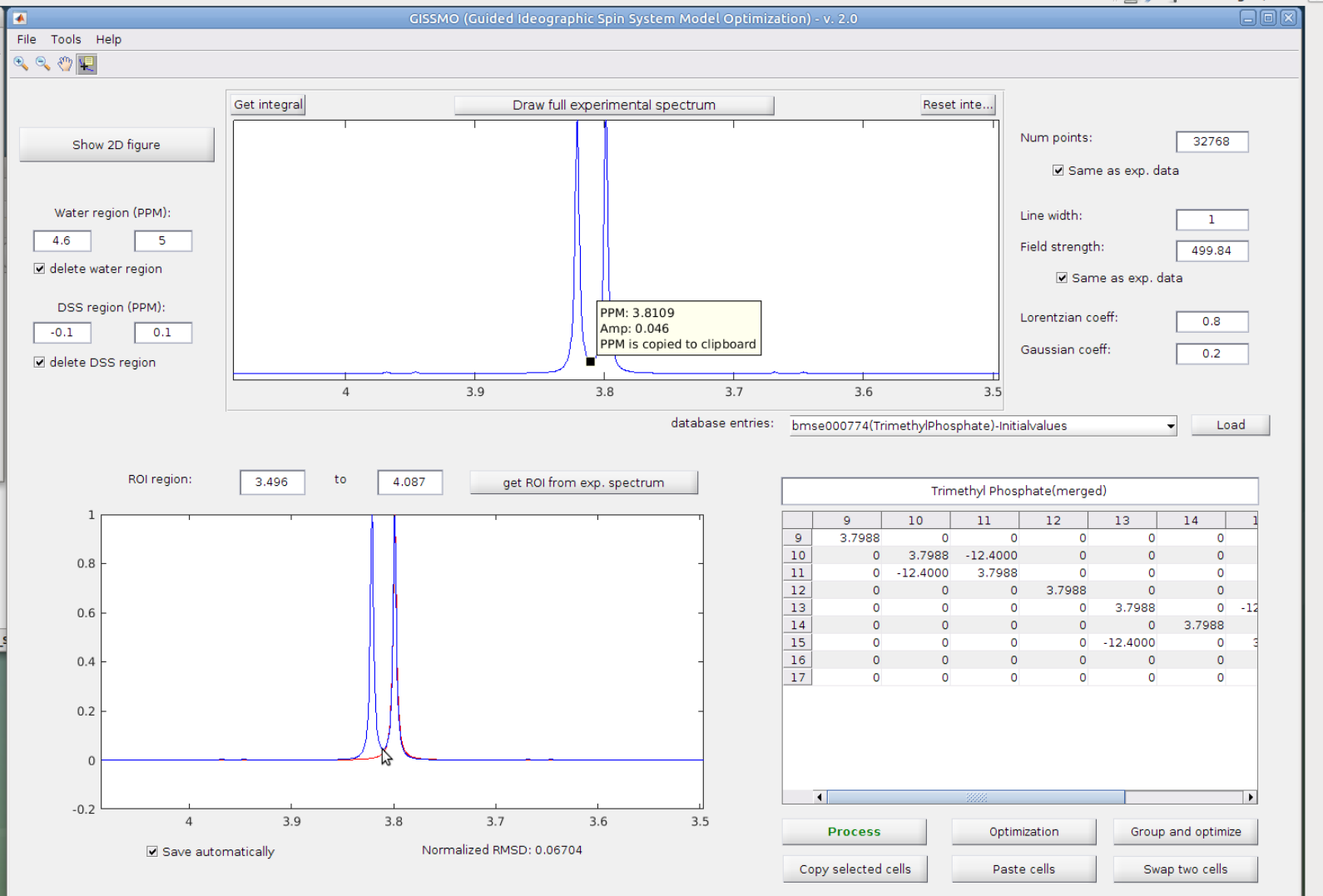
Brow...

\*spin\_s





Network  
Brow...

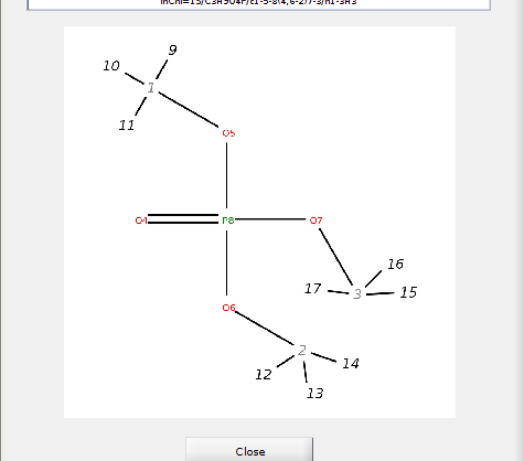


InChI=1S/C3H9O4P/c1-5-8(4,6-2)/7-3/h1-3H3

Get integral

Draw full experimental spectrum

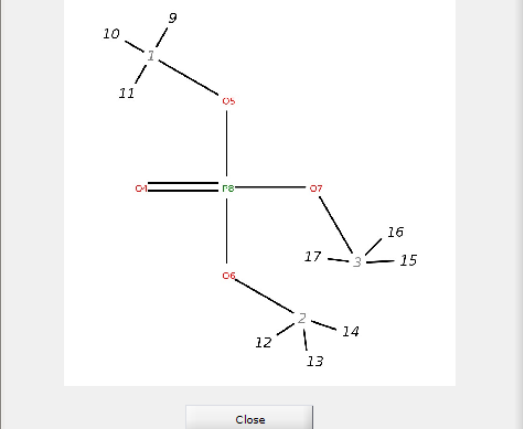
Reset inte...



Show 2D figure

Water region (PPM):

Num points: 32768



4.6 5

☒ delete water region

☒ Same as exp. data

DSS region (PPM):

-0.1 0.1

☒ delete DSS region

Line width: 1

Close

Water region (PPM):

Field strength: 499.84

☒ Same as exp. data

Network

DSS region (PPM):

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Brow...

-0.1 0.1

database entries: bmse000774(TrimethylPhosphate)-Initialvalues

Load

\*spin\_s

☒ delete DSS region

ROI region: 3.496 to 4.087

get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.06704

Trimethyl Phosphate(merged)

Process

Optimization

Group and optimize

Copy selected cells

Paste cells

Swap two cells

PPM: 3.8111

Amp: 0.046

PPM is copied to clipboard

Table with 8 columns: 9, 10, 11, 12, 13, 14, 15, 16, 17

3.8111

0

0

0

3.7988

-12.4000

0

0

-12.4000

3.7988

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3.7988

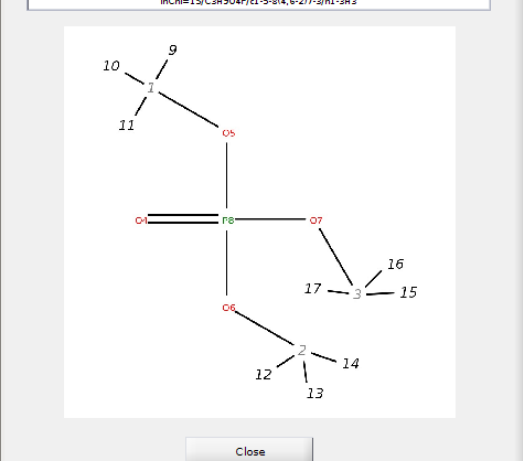
0

InChI=1S/C3H9O4P/c1-5-8(4,6-2)/7-3/h1-3H3

Get integral

Draw full experimental spectrum

Reset inte...



Show 2D figure

Water region (PPM):

Num points: 32768

4.6 5

delete water region

DSS region (PPM):

Same as exp. data

-0.1 0.1

delete DSS region

Line width: 1

Field strength: 499.84

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000774(TrimethylPhosphate)-Initialvalues

Load

ROI region: 3.496 to 4.087

get ROI from exp. spectrum

Repick peak

PPM: 3.8111

Amp: 0.046

PPM is copied to clipboard

Save automatically

Normalized RMSD: 0.06704

Process

Optimization

Group and optimize

Copy selected cells

Paste cells

Swap two cells

Trimethyl Phosphate(merged)

12 13 14 15 16 17

9 0 0 0 0 0 0

10 4000 0 0 0 0 0

11 8111 0 0 0 0 0

12 0 3.8111 0 0 0 0

13 0 0 3.8111 0 -12.4000 0

14 0 0 0 3.8111 0 0

15 0 0 -12.4000 0 3.7988 0

16 0 0 0 0 0 3.8111 -12.4000

17 0 0 0 0 0 -12.4000 3.8111

18 0 0 0 0 0 0 0

19 0 0 0 0 0 0 0

20 0 0 0 0 0 0 0

21 0 0 0 0 0 0 0

22 0 0 0 0 0 0 0

23 0 0 0 0 0 0 0

24 0 0 0 0 0 0 0

25 0 0 0 0 0 0 0

26 0 0 0 0 0 0 0

27 0 0 0 0 0 0 0

28 0 0 0 0 0 0 0

29 0 0 0 0 0 0 0

30 0 0 0 0 0 0 0

31 0 0 0 0 0 0 0

32 0 0 0 0 0 0 0

33 0 0 0 0 0 0 0

34 0 0 0 0 0 0 0

35 0 0 0 0 0 0 0

36 0 0 0 0 0 0 0

37 0 0 0 0 0 0 0

38 0 0 0 0 0 0 0

39 0 0 0 0 0 0 0

40 0 0 0 0 0 0 0

41 0 0 0 0 0 0 0

42 0 0 0 0 0 0 0

43 0 0 0 0 0 0 0

44 0 0 0 0 0 0 0

45 0 0 0 0 0 0 0

46 0 0 0 0 0 0 0

47 0 0 0 0 0 0 0

48 0 0 0 0 0 0 0

49 0 0 0 0 0 0 0

50 0 0 0 0 0 0 0

51 0 0 0 0 0 0 0

52 0 0 0 0 0 0 0

53 0 0 0 0 0 0 0

54 0 0 0 0 0 0 0

55 0 0 0 0 0 0 0

56 0 0 0 0 0 0 0

57 0 0 0 0 0 0 0

58 0 0 0 0 0 0 0

59 0 0 0 0 0 0 0

60 0 0 0 0 0 0 0

61 0 0 0 0 0 0 0

62 0 0 0 0 0 0 0

63 0 0 0 0 0 0 0

64 0 0 0 0 0 0 0

65 0 0 0 0 0 0 0

66 0 0 0 0 0 0 0

67 0 0 0 0 0 0 0

68 0 0 0 0 0 0 0

69 0 0 0 0 0 0 0

70 0 0 0 0 0 0 0

71 0 0 0 0 0 0 0

72 0 0 0 0 0 0 0

73 0 0 0 0 0 0 0

74 0 0 0 0 0 0 0

75 0 0 0 0 0 0 0

76 0 0 0 0 0 0 0

77 0 0 0 0 0 0 0

78 0 0 0 0 0 0 0

79 0 0 0 0 0 0 0

80 0 0 0 0 0 0 0

81 0 0 0 0 0 0 0

82 0 0 0 0 0 0 0

83 0 0 0 0 0 0 0

84 0 0 0 0 0 0 0

85 0 0 0 0 0 0 0

86 0 0 0 0 0 0 0

87 0 0 0 0 0 0 0

88 0 0 0 0 0 0 0

89 0 0 0 0 0 0 0

90 0 0 0 0 0 0 0

91 0 0 0 0 0 0 0

92 0 0 0 0 0 0 0

93 0 0 0 0 0 0 0

94 0 0 0 0 0 0 0

95 0 0 0 0 0 0 0

96 0 0 0 0 0 0 0

97 0 0 0 0 0 0 0

98 0 0 0 0 0 0 0

99 0 0 0 0 0 0 0

100 0 0 0 0 0 0 0

101 0 0 0 0 0 0 0

102 0 0 0 0 0 0 0

103 0 0 0 0 0 0 0

104 0 0 0 0 0 0 0

105 0 0 0 0 0 0 0

106 0 0 0 0 0 0 0

107 0 0 0 0 0 0 0

108 0 0 0 0 0 0 0

109 0 0 0 0 0 0 0

110 0 0 0 0 0 0 0

111 0 0 0 0 0 0 0

112 0 0 0 0 0 0 0

113 0 0 0 0 0 0 0

114 0 0 0 0 0 0 0

115 0 0 0 0 0 0 0

116 0 0 0 0 0 0 0

117 0 0 0 0 0 0 0

118 0 0 0 0 0 0 0

119 0 0 0 0 0 0 0

120 0 0 0 0 0 0 0

121 0 0 0 0 0 0 0

122 0 0 0 0 0 0 0

123 0 0 0 0 0 0 0

124 0 0 0 0 0 0 0

125 0 0 0 0 0 0 0

126 0 0 0 0 0 0 0

127 0 0 0 0 0 0 0

128 0 0 0 0 0 0 0

129 0 0 0 0 0 0 0

130 0 0 0 0 0 0 0

131 0 0 0 0 0 0 0

132 0 0 0 0 0 0 0

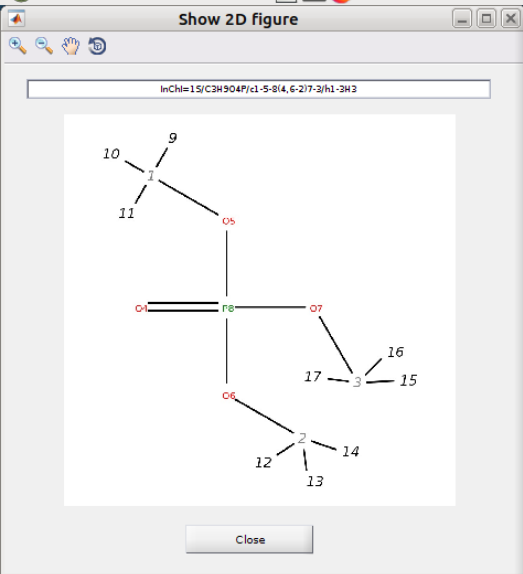
133 0 0 0 0 0 0 0

134 0 0 0 0 0 0 0

135 0 0 0 0 0 0 0

136 0 0 0 0 0 0 0

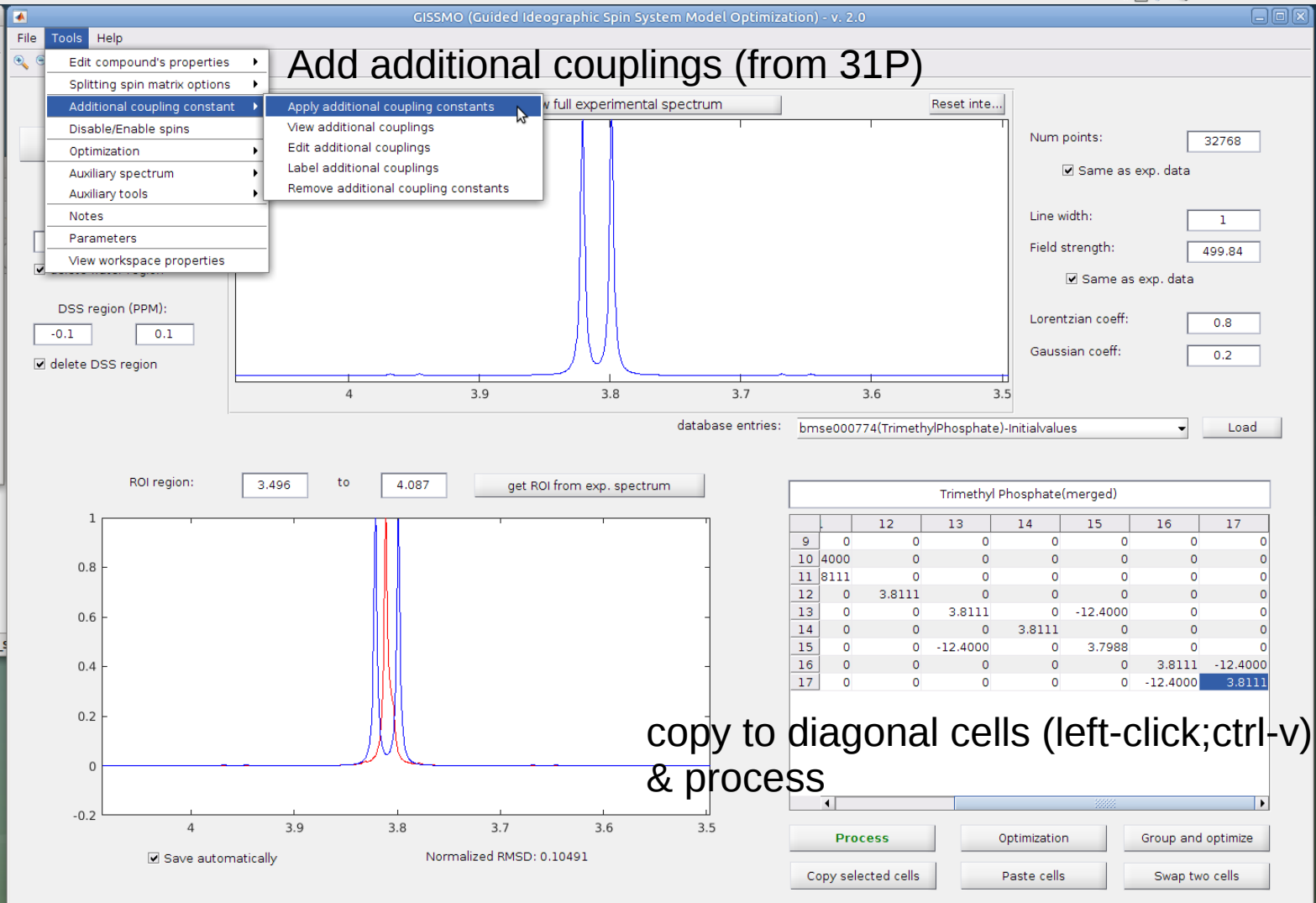


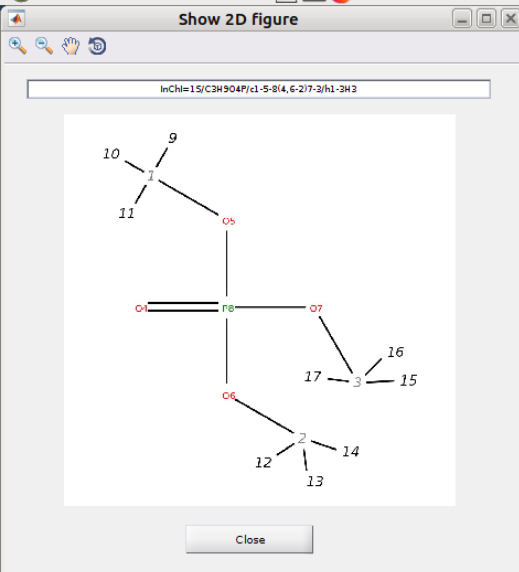


Network

Brow...

\*spin\_s

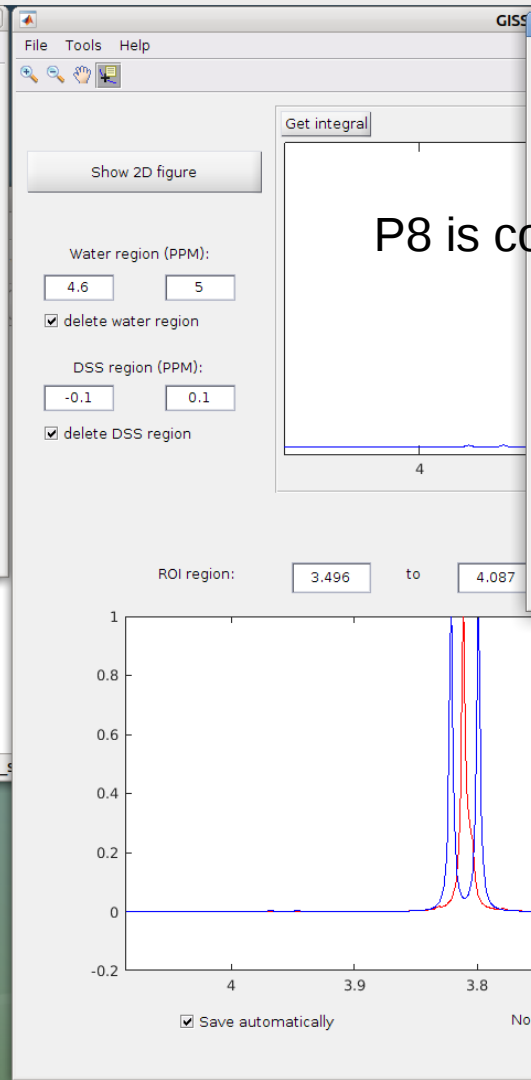




Network

Brow...

\*spin\_s



Apply different additional couplings to different spin groups

Number of groups of spins: 2

Total number of additional couplings: 2

Create

Apply

Cancel

P8 is coupled to all 9 (identical) methyl protons

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

Show 2D figure

InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3

Close

Network

Brow...

\*spin\_s

File Tools Help

Get integral

Show 2D figure

Water region (PPM):  
4.6 5  
☒ delete water region

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

ROI region: 3.496 to 4.087

☒ Save automatically

Normalized RMSD: 0.10491

Apply different additional couplings to different spin groups

Number of groups of spins: 1

Total number of additional couplings: 1

Create

Apply

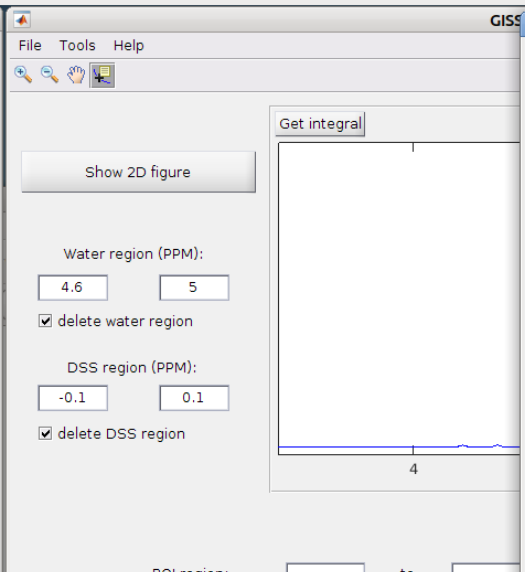
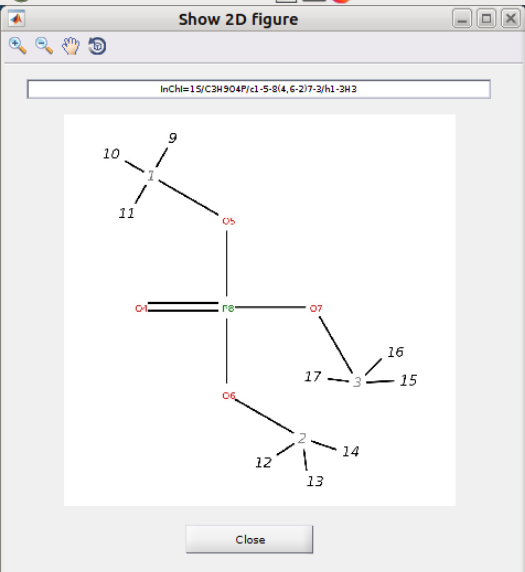
Cancel

The methyl protons make 1 group of spins  
And there is 1 coupling constant to that group

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells



Apply different additional couplings to different spin groups

Number of groups of spins: 1  
Total number of additional couplings: 1

Create

Select spins

Spin names	Group ID
1 9	select
2 10	select
3 11	group(1)
4 12	select
5 13	select
6 14	select
7 15	select
8 16	select
9 17	select

Additional couplings

Coupling constant	Group ID
1	select

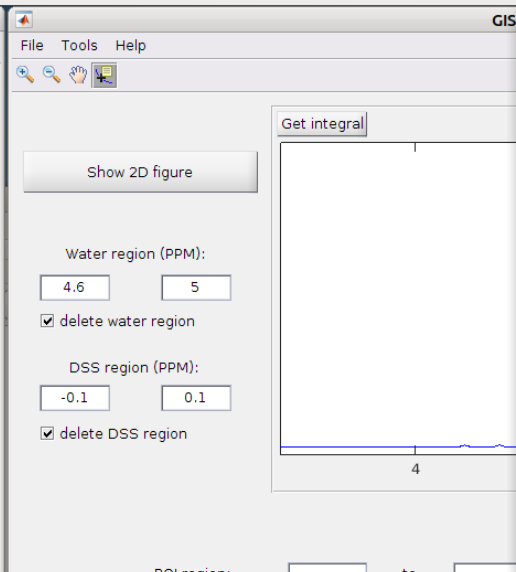
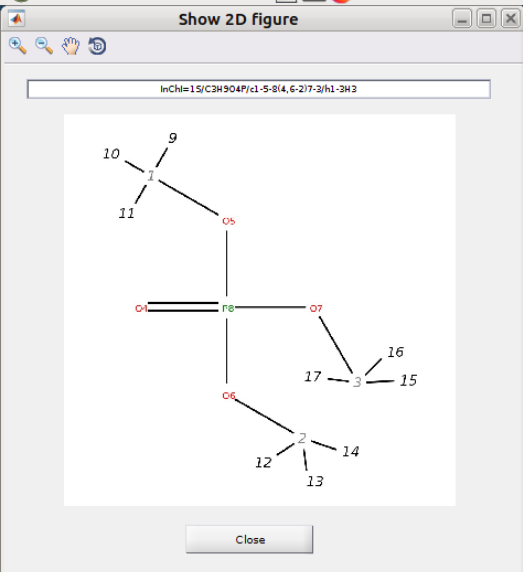
Set all protons to group 1

Apply Cancel

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells



Apply different additional couplings to different spin groups

Number of groups of spins: 1

Total number of additional couplings: 1

Create

Select spins

Spin names	Group ID
1 9	group(1)
2 10	group(1)
3 11	group(1)
4 12	group(1)
5 13	group(1)
6 14	group(1)
7 15	group(1)
8 16	group(1)
9 17	group(1)

Additional couplings

Coupling constant	Group ID
1	select
	group(1)

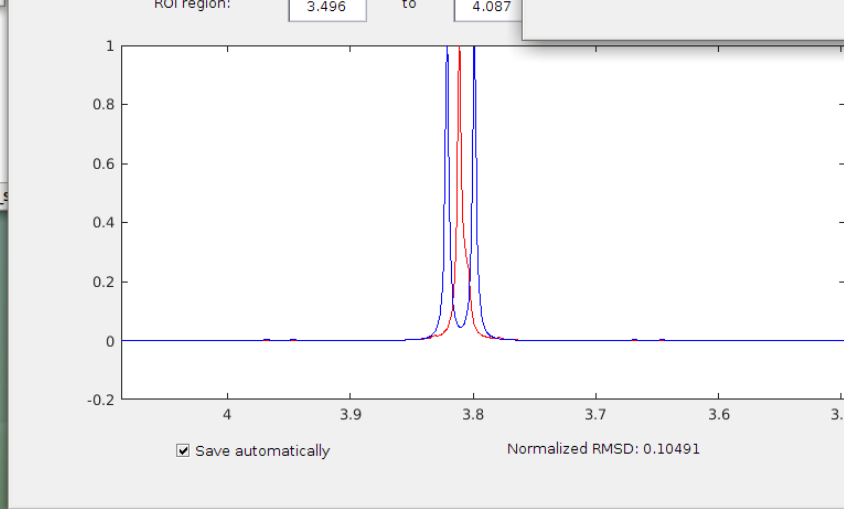
Set coupling constant to group 1

Apply Cancel

Network

Brow...

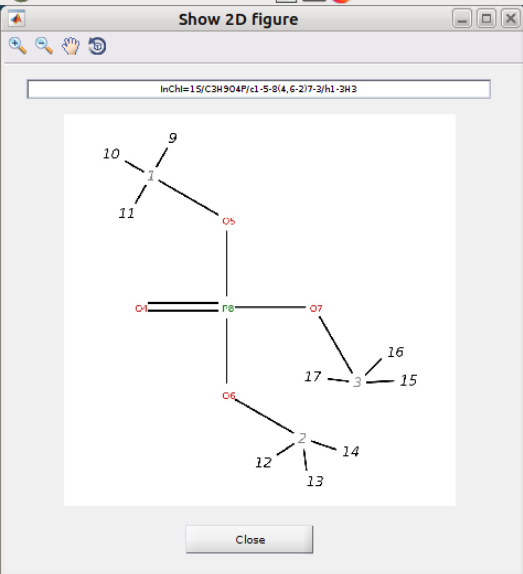
\*spin\_s



	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

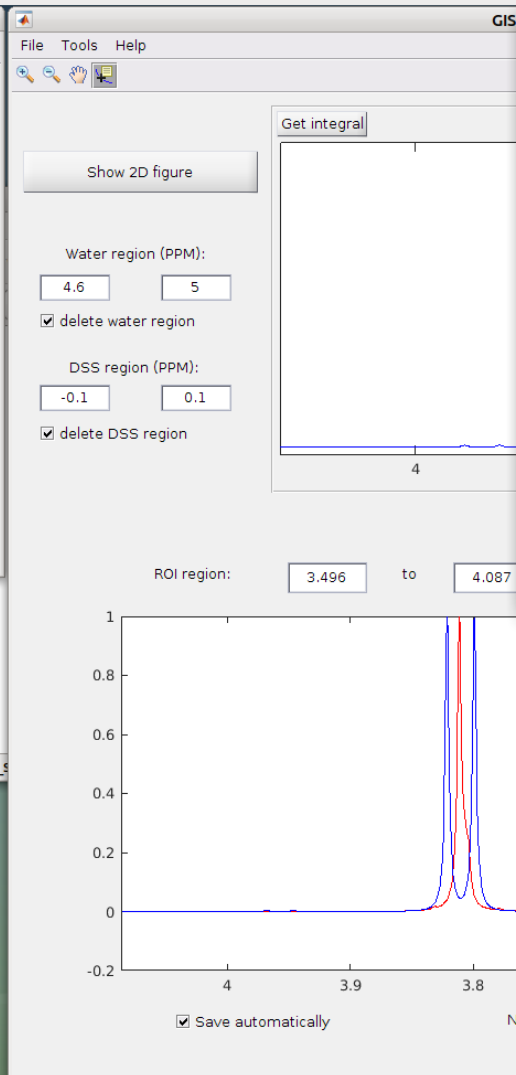
Copy selected cells Paste cells Swap two cells



Network

Brow...

\*spin\_s



Apply different additional couplings to different spin groups

Number of groups of spins: 1

Total number of additional couplings: 1

Create

Select spins

Spin names	Group ID
1 9	group(1)
2 10	group(1)
3 11	group(1)
4 12	group(1)
5 13	group(1)
6 14	group(1)
7 15	group(1)
8 16	group(1)
9 17	group(1)

Additional couplings

Coupling constant	Group ID
1 7	group(1)

Estimate coupling ~7Hz

Apply

Cancel

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

Show 2D figure

InChI=1S/C3H9O4P/c1-5-8(4,6-2)7-3/h1-3H3

Close

File Tools Help

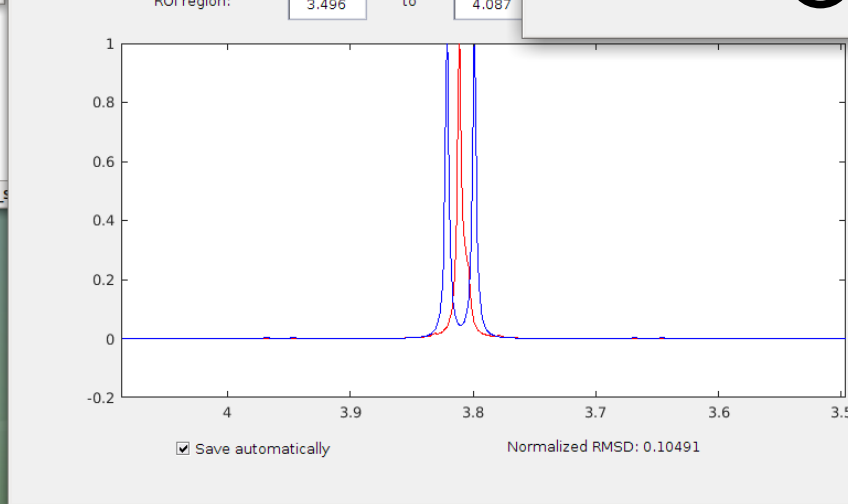
Get integral

Show 2D figure

Water region (PPM):  
4.6 5  
☒ delete water region

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

ROI region: 3.496 to 4.087



Apply different additional couplings to different spin groups

Number of groups of spins: 1  
Total number of additional couplings: 1  
Create

Select spins

Spin names	Group ID
1 9	group(1)
2 10	group(1)
3 11	group(1)
4 12	group(1)
5 13	group(1)
6 14	group(1)
7 15	group(1)
8 16	group(1)
9 17	group(1)

Additional couplings

Coupling constant	Group ID
1 7	group(1)

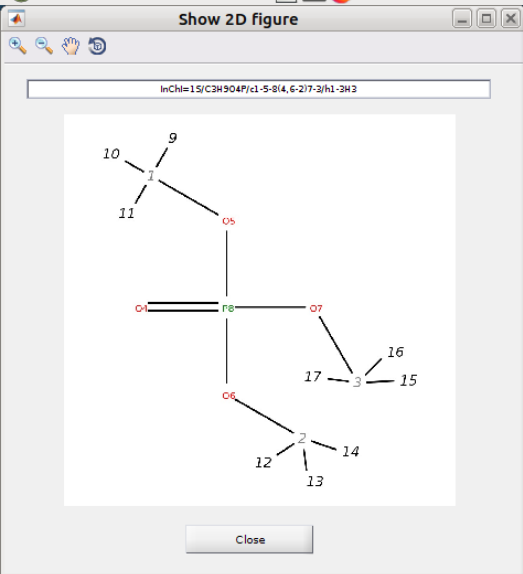
Apply

Cancel

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	0	3.8111
17	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

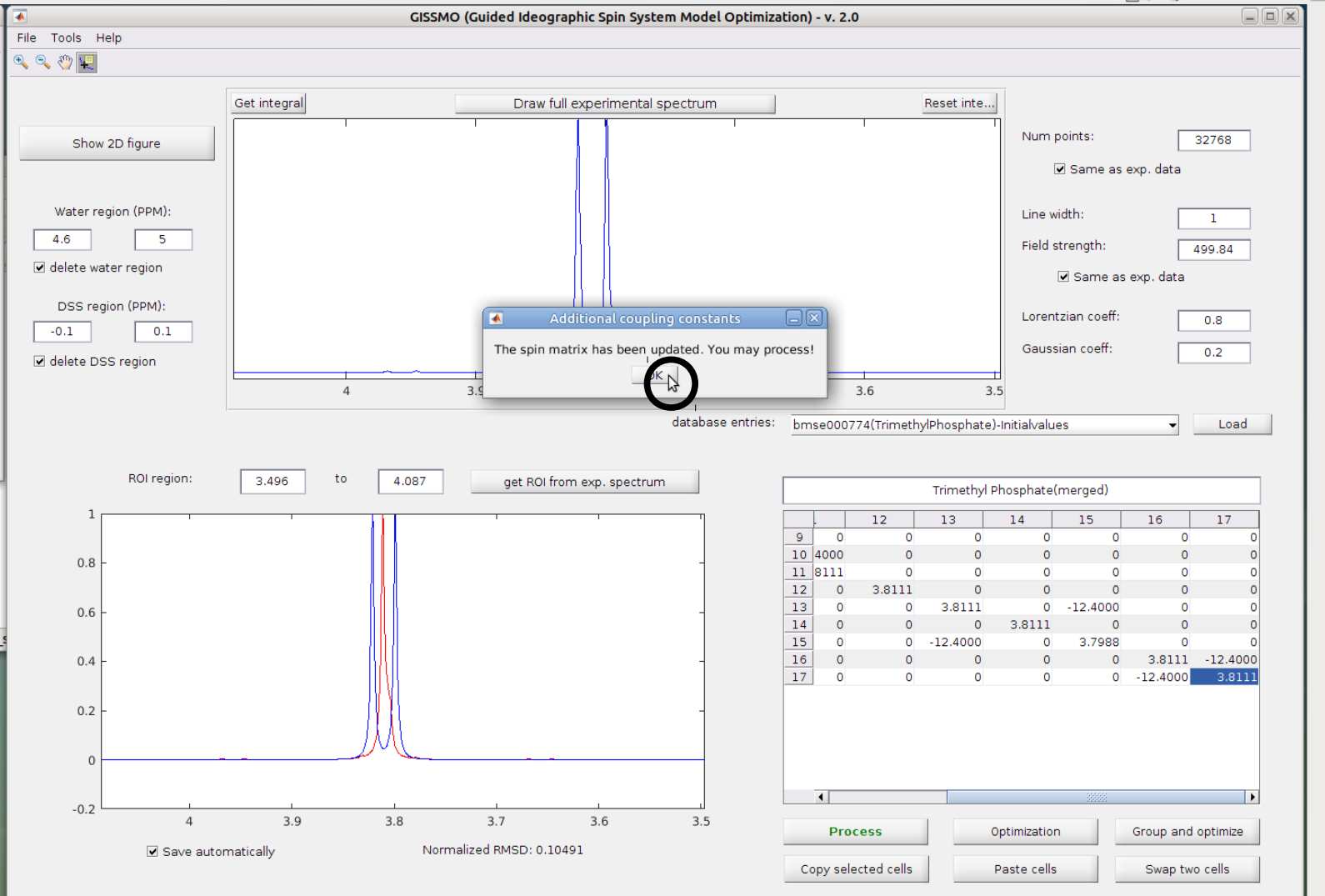
Copy selected cells Paste cells Swap two cells



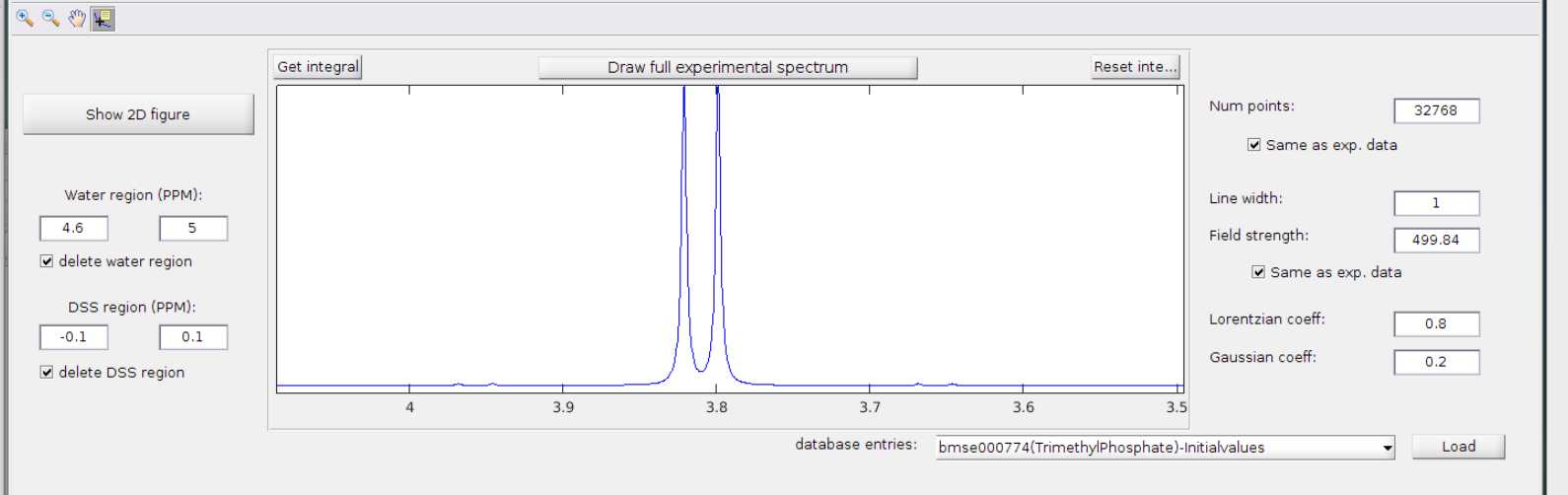
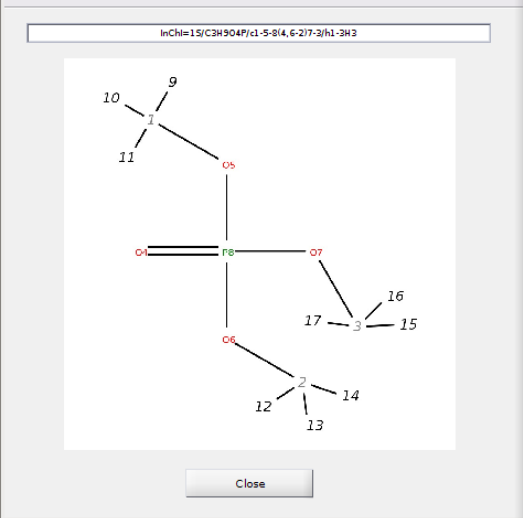
Network

Brow...

\*spin\_s



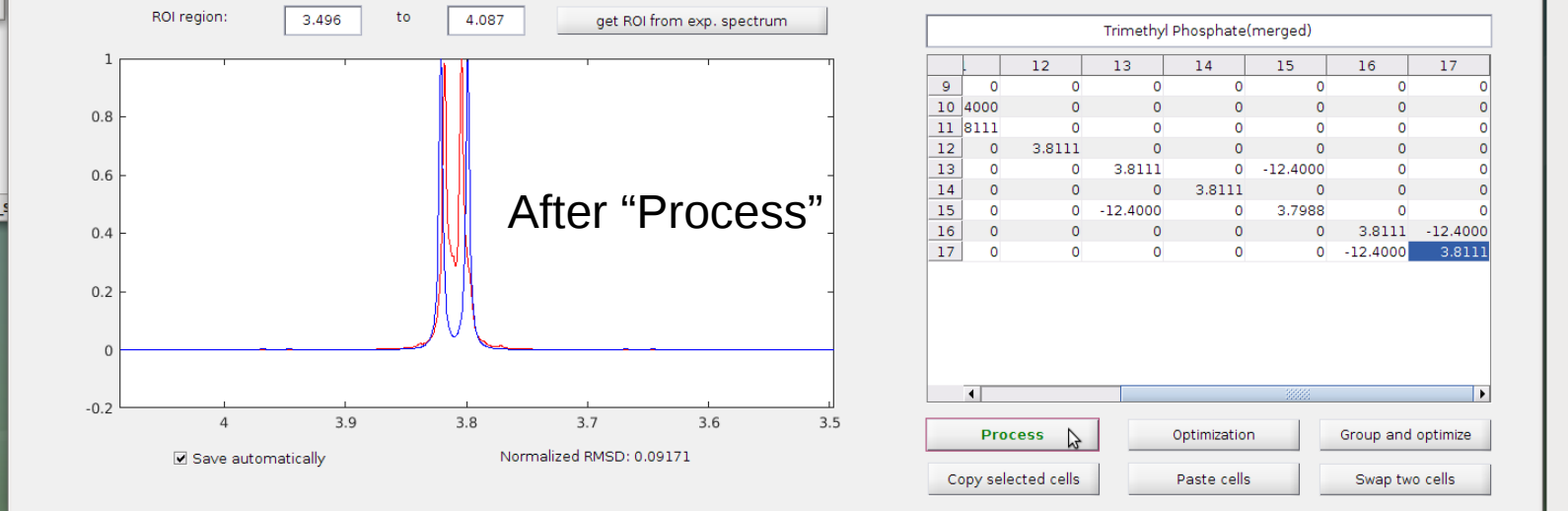


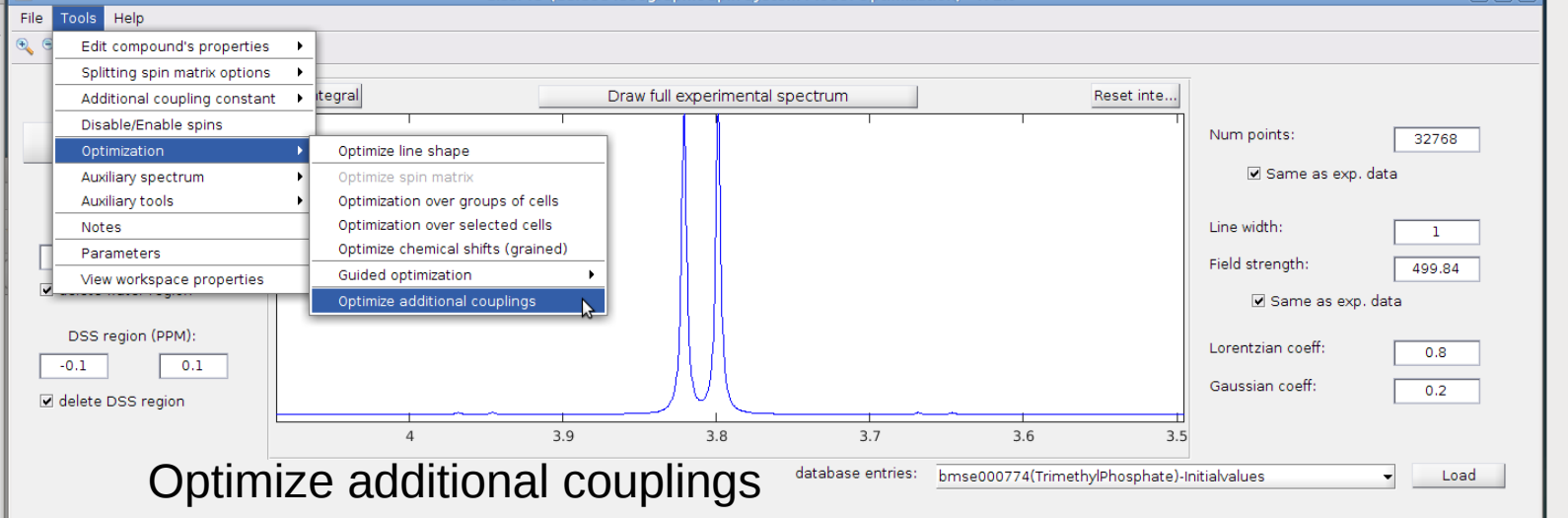
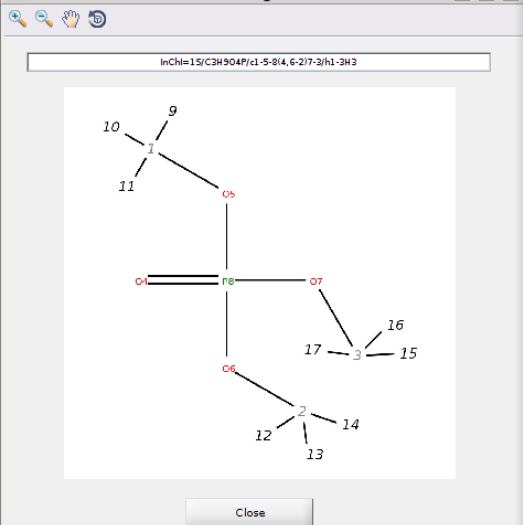


Network

Brow...

\*spin\_s





Network

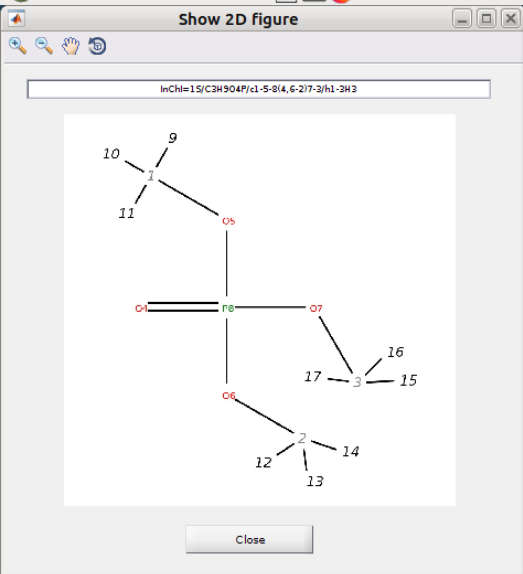
Brow...

\*spin\_s

Trimethyl Phosphate(merged)							
	12	13	14	15	16	17	
9	0	0	0	0	0	0	0
10	4000	0	0	0	0	0	0
11	8111	0	0	0	0	0	0
12	0	3.8111	0	0	0	0	0
13	0	0	3.8111	0	-12.4000	0	0
14	0	0	0	3.8111	0	0	0
15	0	0	-12.4000	0	3.7988	0	0
16	0	0	0	0	0	3.8111	-12.4000
17	0	0	0	0	0	-12.4000	3.8111

Process Optimization Group and optimize

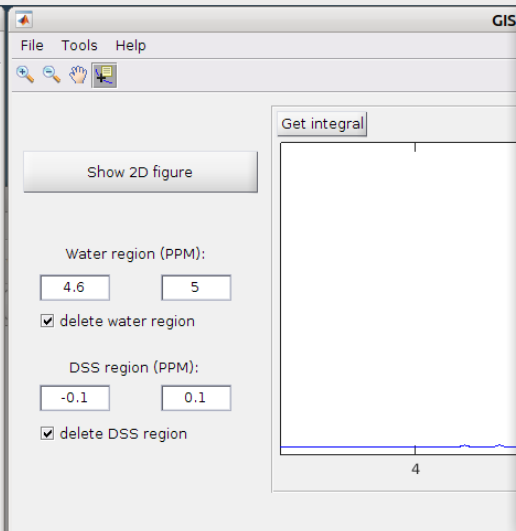
Copy selected cells Paste cells Swap two cells



Network

Brow...

\*spin\_s



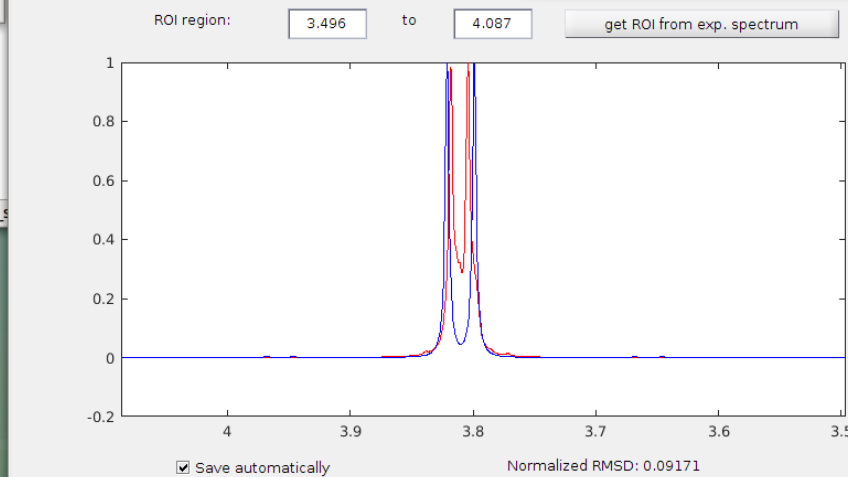
choose additional couplings for optimization

Choose additional couplings to be optimized

	spins	coupling constant	spin groups ID	coupling groups ID	optimize	keep va
1	9,10,11,1...	7	group(1)	group(1)	<input checked="" type="checkbox"/>	group(1)

Ok

Cancel



Trimethyl Phosphate(merged)

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	3.8111	-12.4000
17	0	0	0	0	-12.4000	3.8111

Process

Optimization

Group and optimize

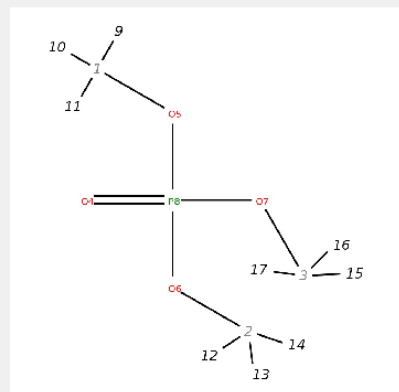
Copy selected cells

Paste cells

Swap two cells

# Show 2D figure

InChI=1S/C3H9O4P/c1-5-8(4,6-2)/7-3/h1-3H3



Close

## Network

Brow...

\*spin\_s

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

File Tools Help



Show 2D figure

Water region (PPM):

4.6 5

☒ delete water region

DSS region (PPM):

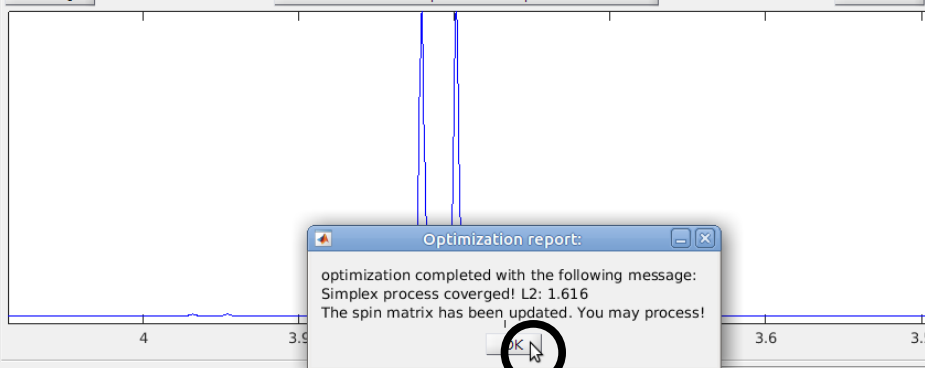
-0.1 0.1

☒ delete DSS region

Get integral

Draw full experimental spectrum

Reset inte...



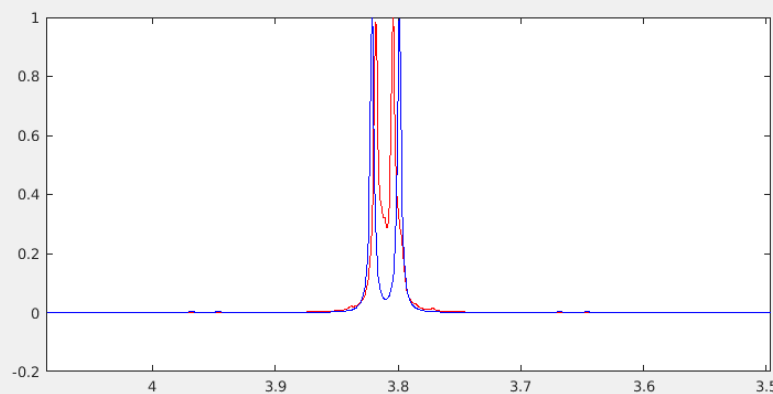
## Optimization report:

optimization completed with the following message:  
Simplex process covered! L2: 1.616  
The spin matrix has been updated. You may process!



ROI region: 3.496 to 4.087

get ROI from exp. spectrum



☒ Save automatically

Normalized RMSD: 0.09171

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: bmse000774(TrimethylPhosphate)-Initialvalues

Load

## Trimethyl Phosphate(merged)

	12	13	14	15	16	17
9	0	0	0	0	0	0
10	4000	0	0	0	0	0
11	8111	0	0	0	0	0
12	0	3.8111	0	0	0	0
13	0	0	3.8111	0	-12.4000	0
14	0	0	0	3.8111	0	0
15	0	0	-12.4000	0	3.7988	0
16	0	0	0	0	3.8111	-12.4000
17	0	0	0	0	-12.4000	3.8111

Process

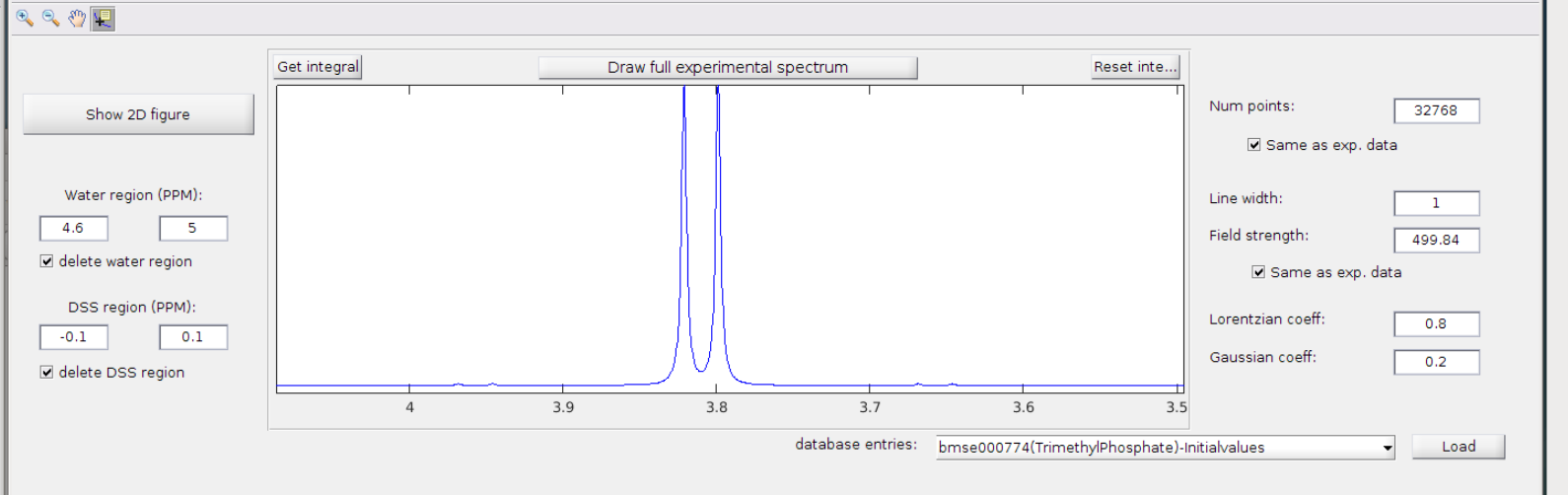
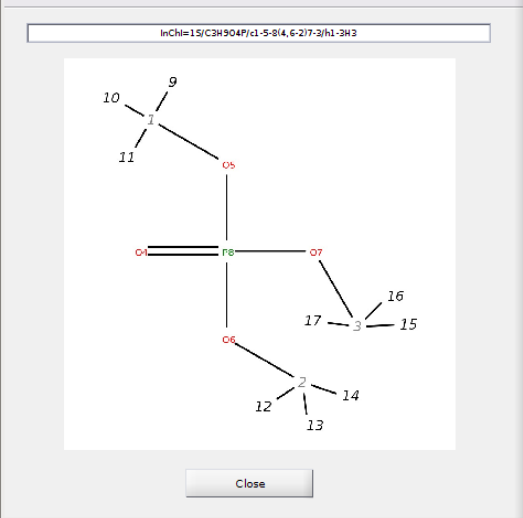
Optimization

Group and optimize

Copy selected cells

Paste cells

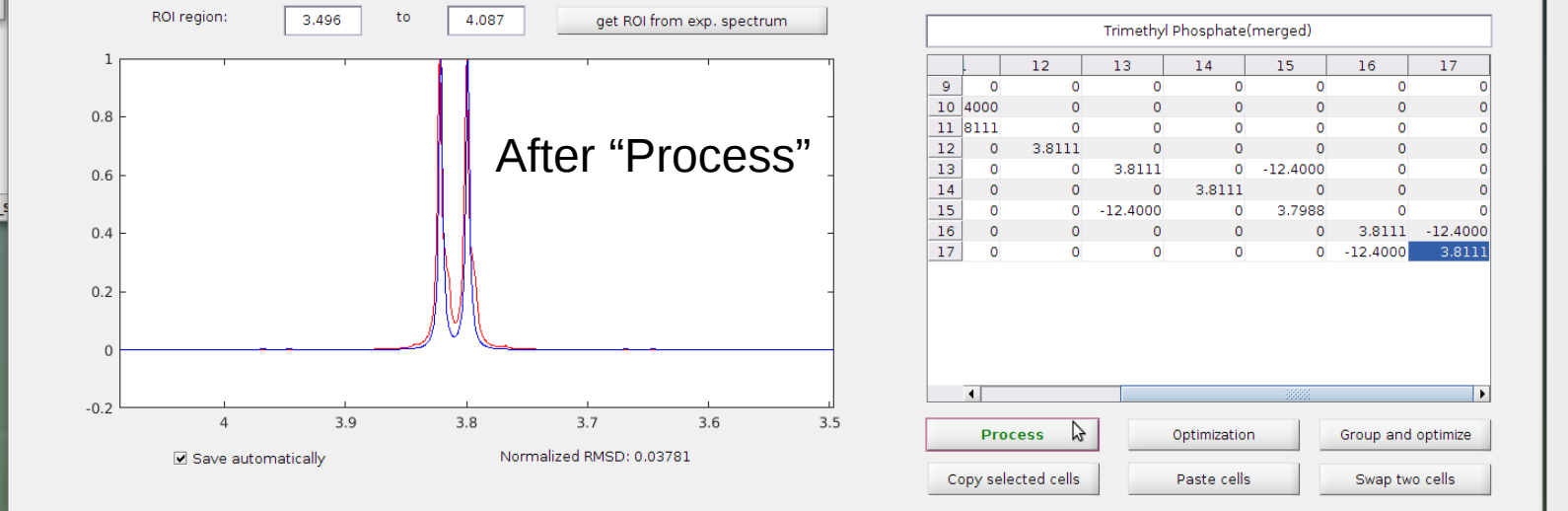
Swap two cells



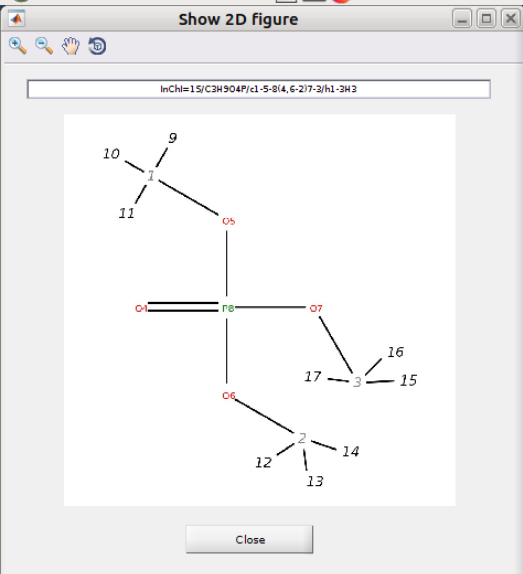
Network

Brow...

\*spin\_s



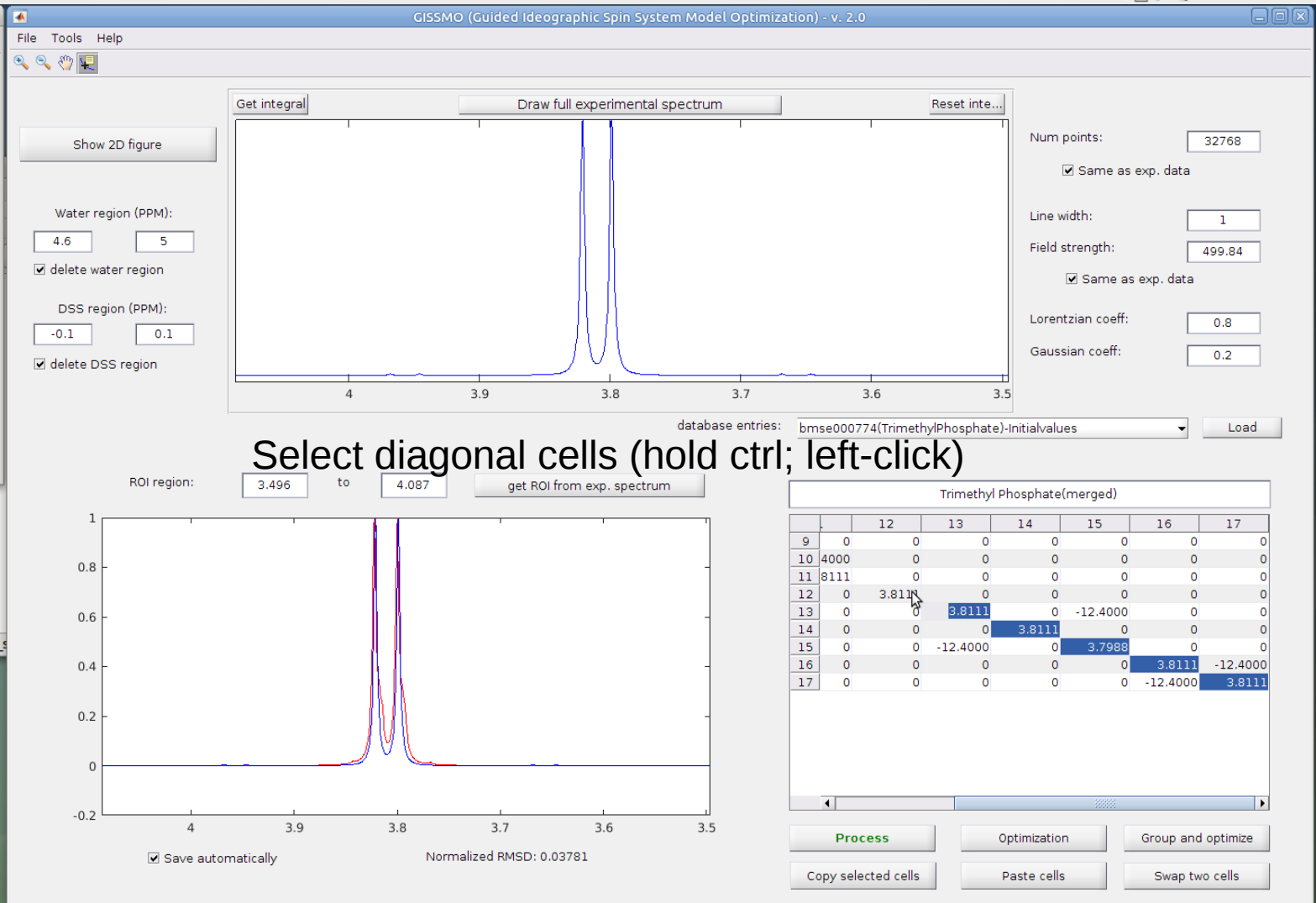


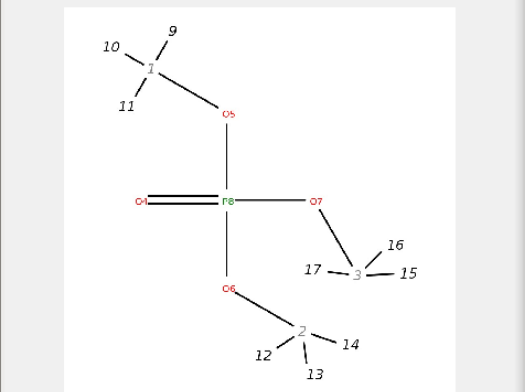
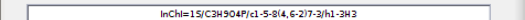


Network

Brow...

\*spin\_s





[Close](#)

	Network	
--	---------	--

 ... 
 
  
 **Brow...**

"spin

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

Get integral

Get integral Draw full experimental spectrum Reset inte...

Num points:	32768
-------------	-------

☒ Same as exp. data

Line width: 1

Field strength: 499.84

☒ Same as exp. data

Lorentzian coeff: 0.8

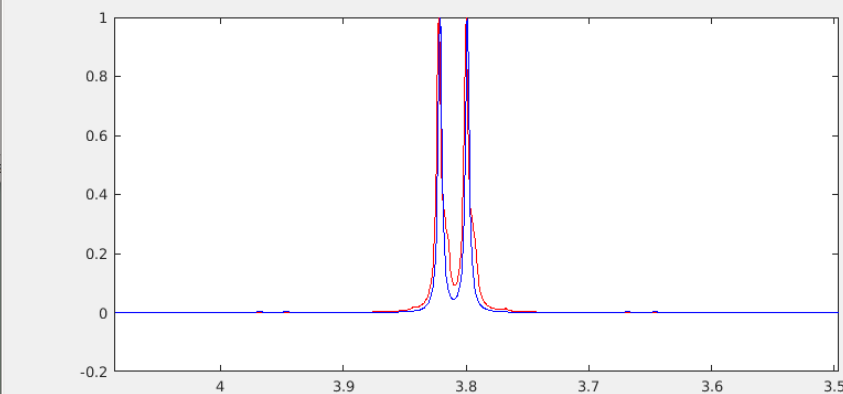
Gaussian coeff: 0.2

database entries: [bmse000774\(TrimethylPhosphate\)-Initialvalues](#)

database entries:

ROI region: 3.496 to 4.087 

ROI region:	3.496	to	4.087	get ROI from exp. spectrum
-------------	-------	----	-------	----------------------------

☒ Save automatically☒ Save automatically Normalized RMSD: 0.03781

Trimethyl Phosphate(merged)

	9	10	11	12	13	14	
9	3.8111	0	0	0	0	0	
10	0	3.8111	-12.4000	0	0	0	
11	0	-12.4000	3.8111	0	0	0	
12	0	0	0	3.8111	0	0	
13	0	0	0	0	3.8111	0	-1
14	0	0	0	0	0	3.8111	
15	0	0	0	0	-12.4000	0	
16	0	0	0	0	0	0	
17	0	0	0	0	0	0	

## Group & optimize

### Process

Process	Optimization
---------	--------------

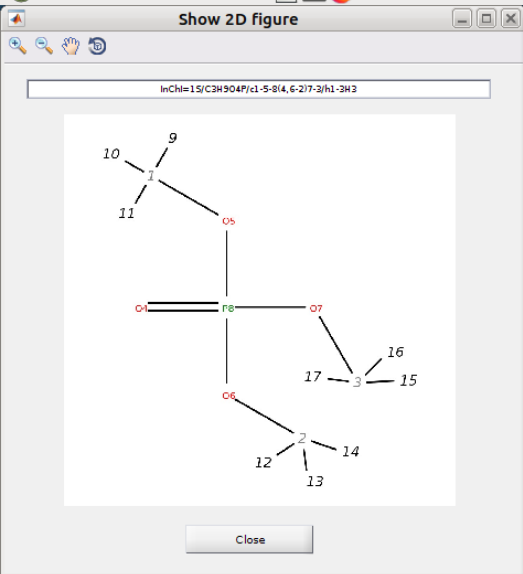
Process	Optimization	Group and optimize
---------	--------------	--------------------

Copy selected cells

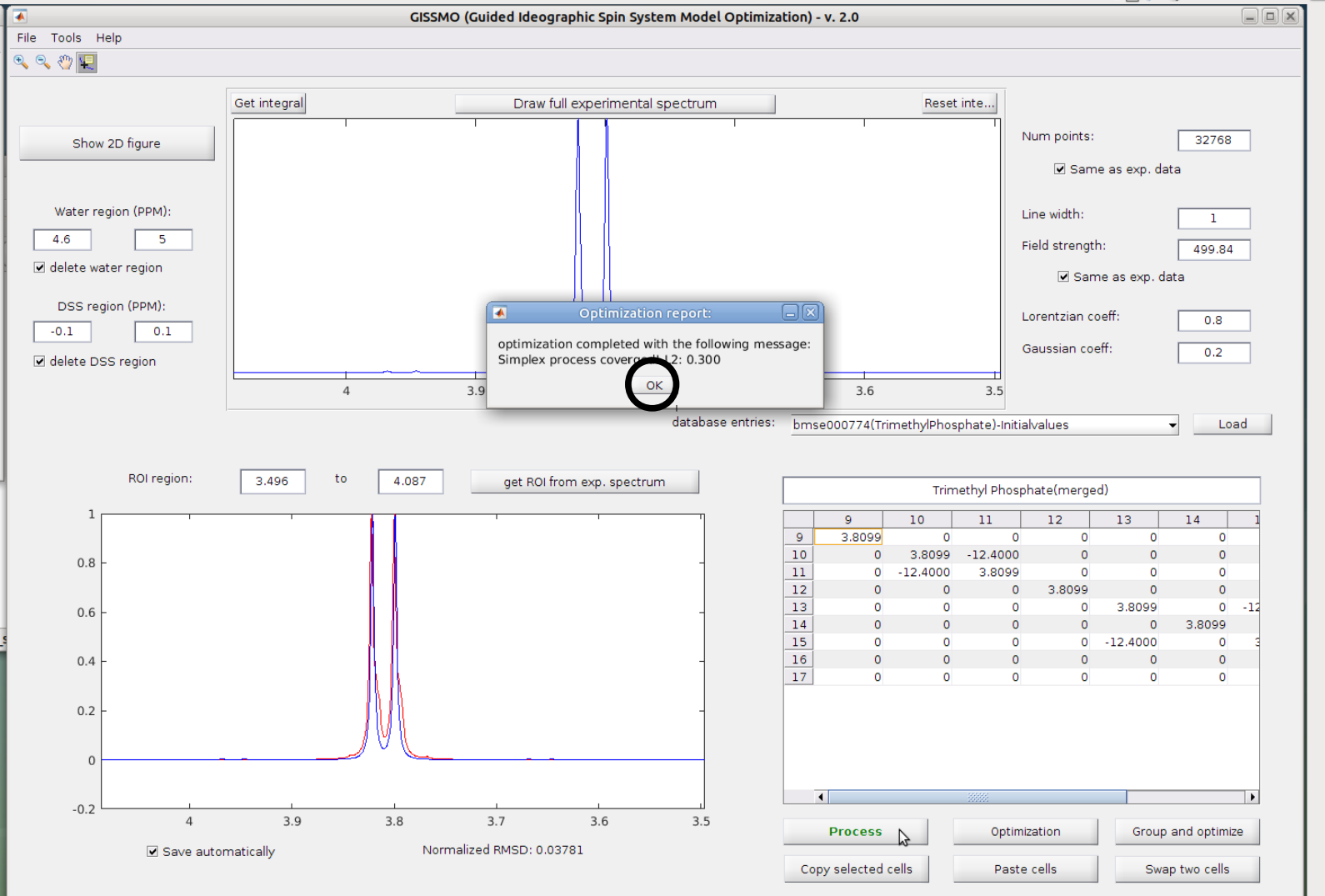
Copy selected cells

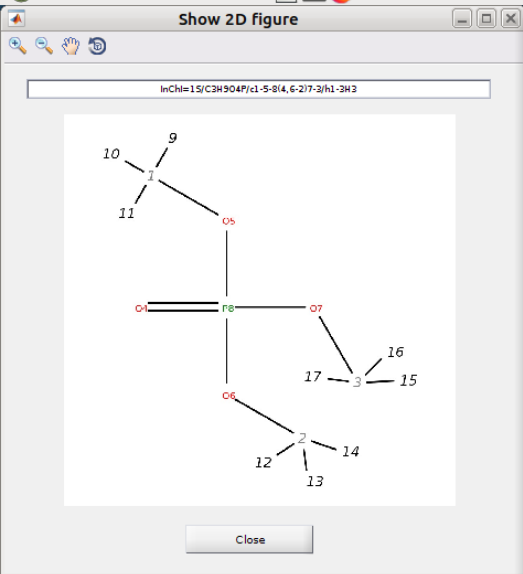
Copy selected cells      Paste cells      Swap two cells





Network  
Brow...

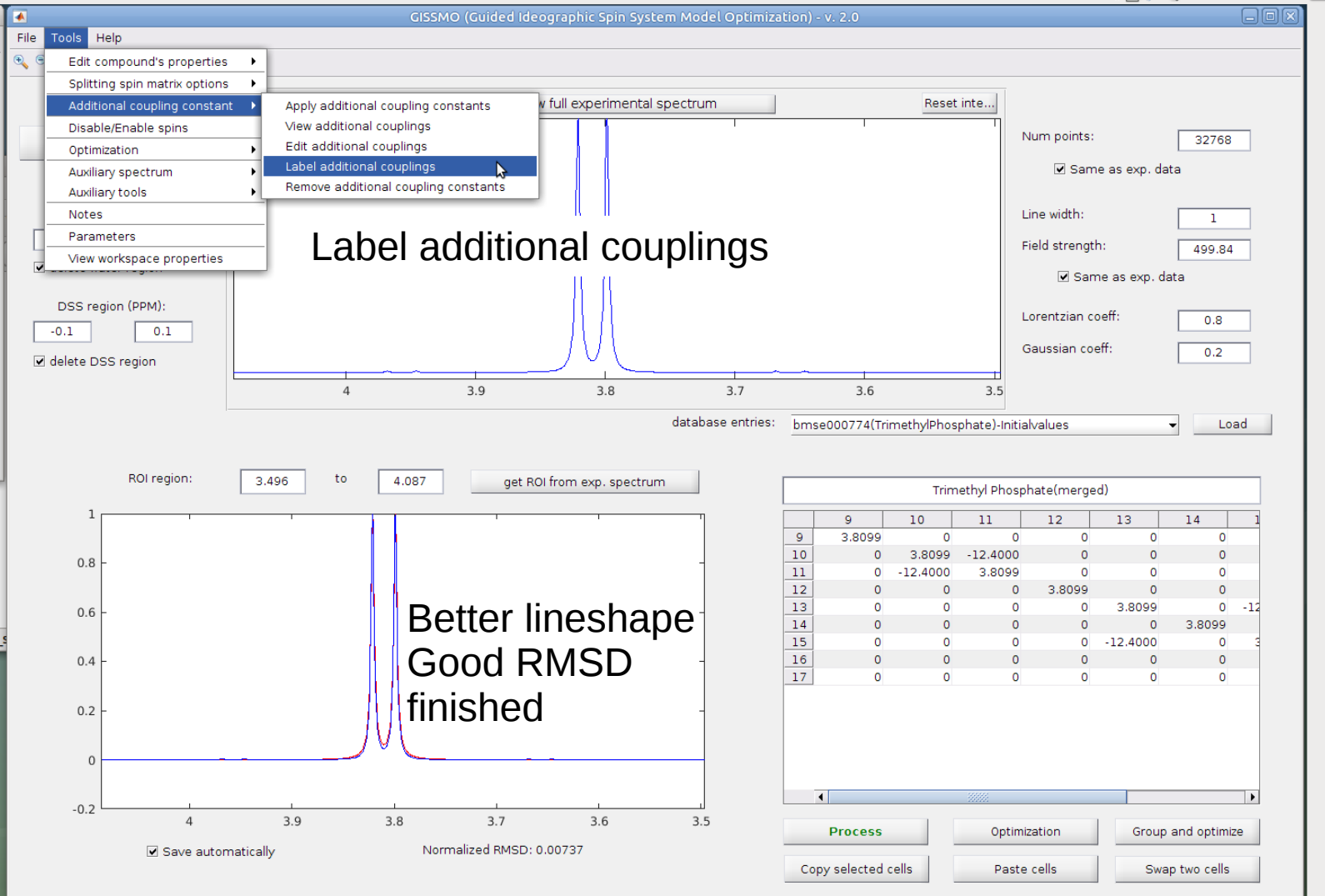


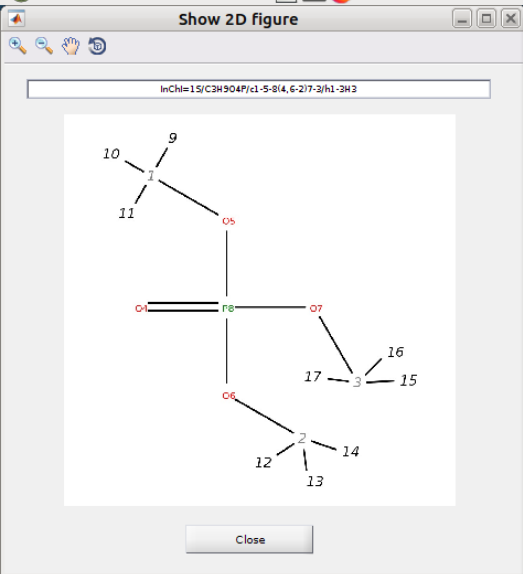


Network

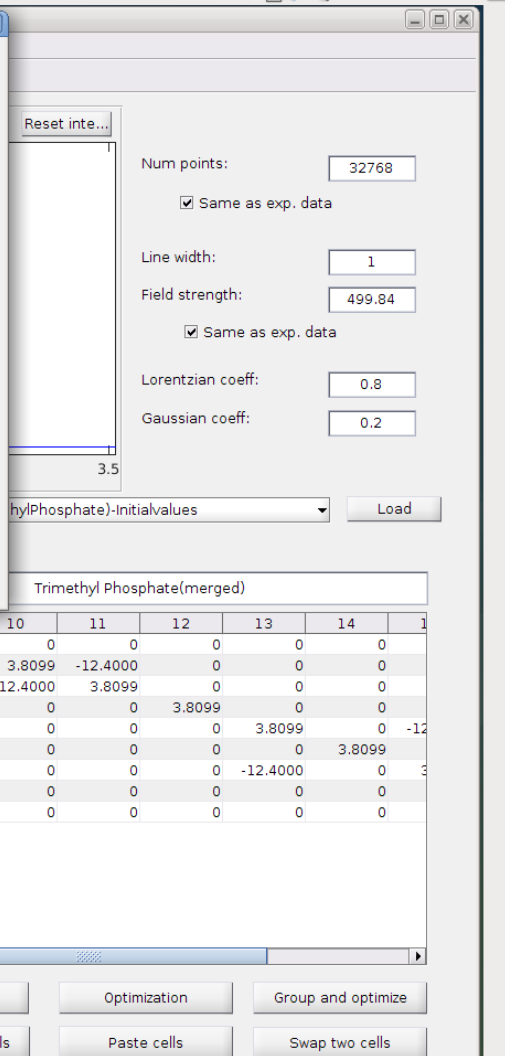
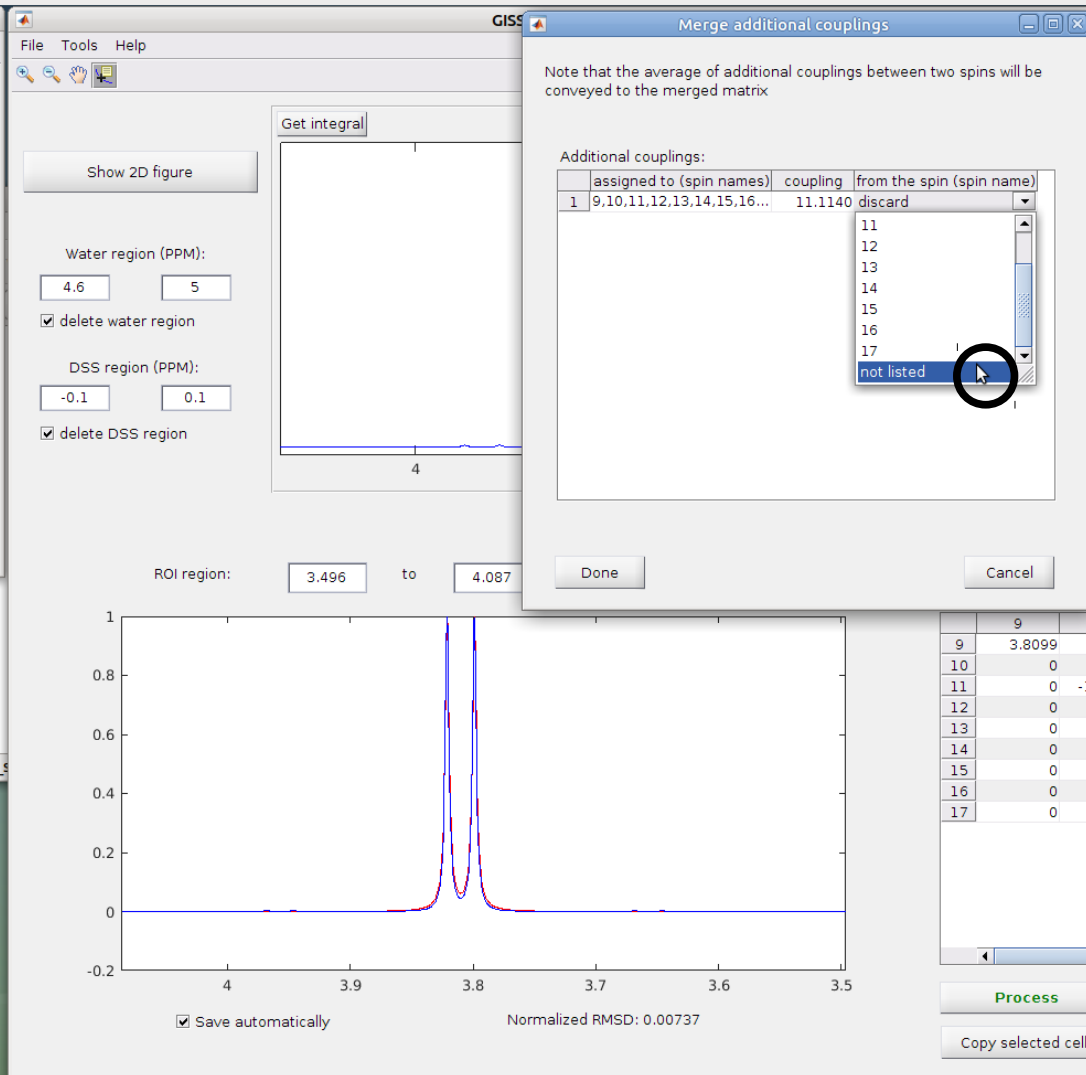
Brow...

\*spin\_s





Network  
Brow...



### Merge additional couplings



File Tools Help

Get integral

4.6 5

DSS region (PPM):

ROI region: 3.496 to 4.087

Additional couplings:

1.140 not listed

Num points: 32768

Line width: 1

Field strength: 499.84

☒ Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

### hylPhosphate)-Initialvalues

Trimethyl Phosphate(merged)

	9	10	11	12	13	14	
9	3.8099	0	0	0	0	0	
10	0	3.8099	-12.4000	0	0	0	
11	0	-12.4000	3.8099	0	0	0	
12	0	0	0	3.8099	0	0	
13	0	0	0	0	3.8099	0	-1
14	0	0	0	0	0	3.8099	
15	0	0	0	0	-12.4000	0	
16	0	0	0	0	0	0	
17	0	0	0	0	0	0	

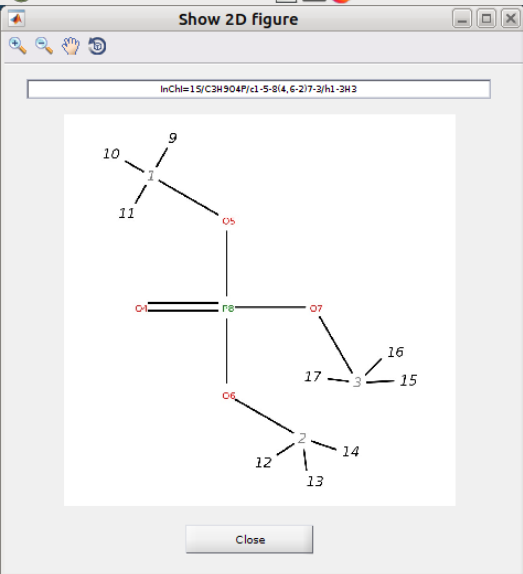
Group and optimize

### Swap two cells

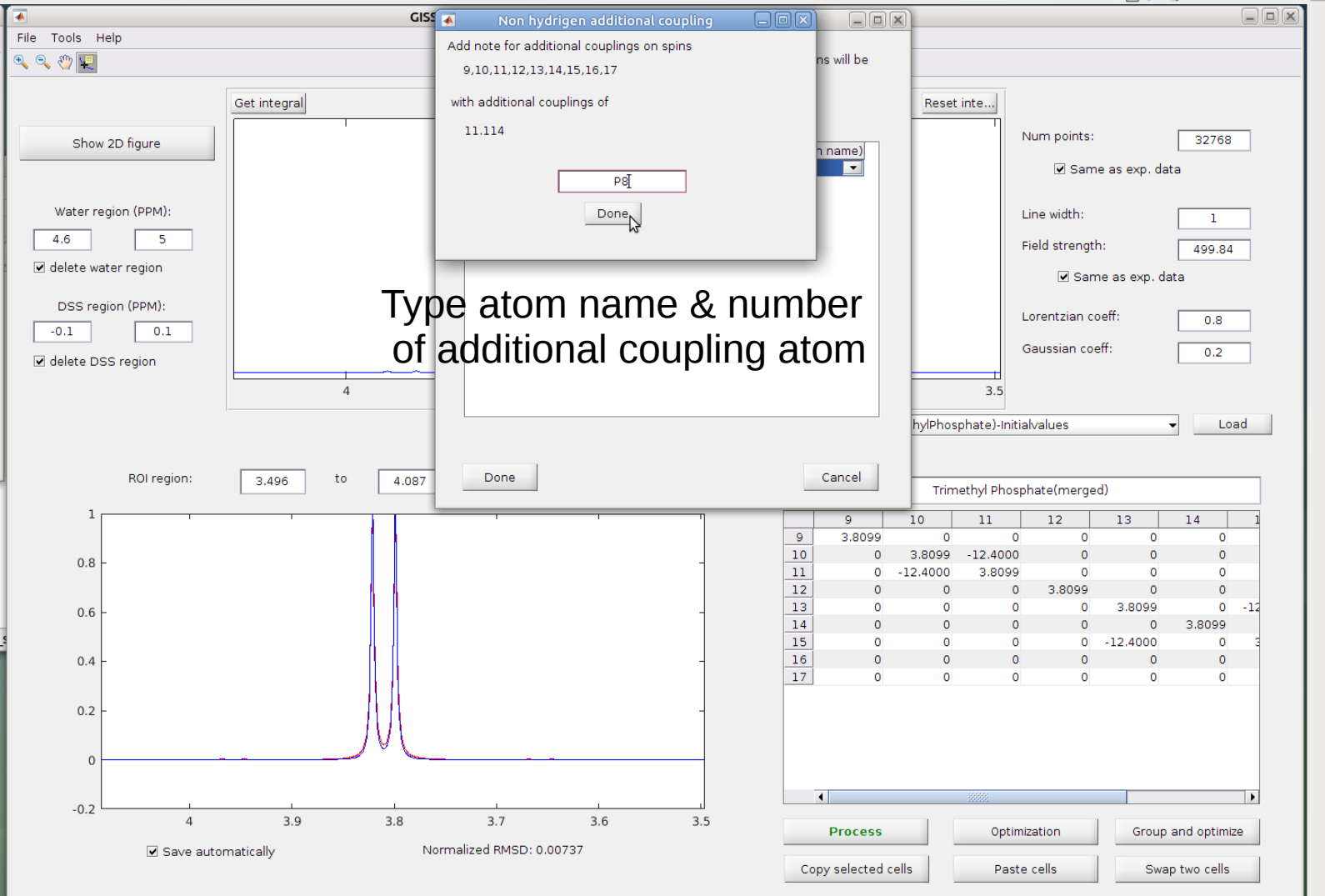
Normalized RMSD: 0.00737

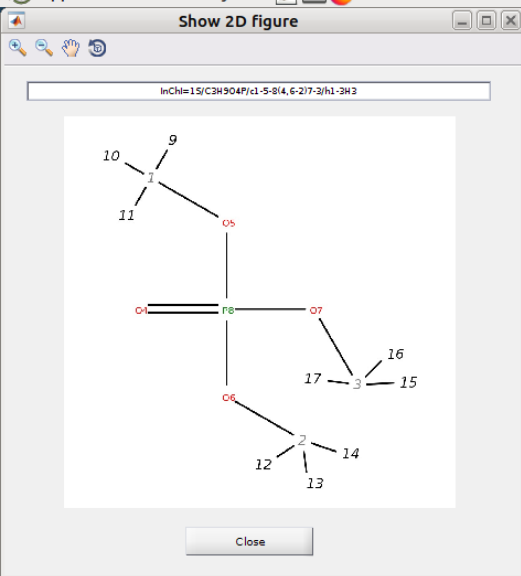
 ...   
 **Brow...**

"spin s



Network  
Brow...

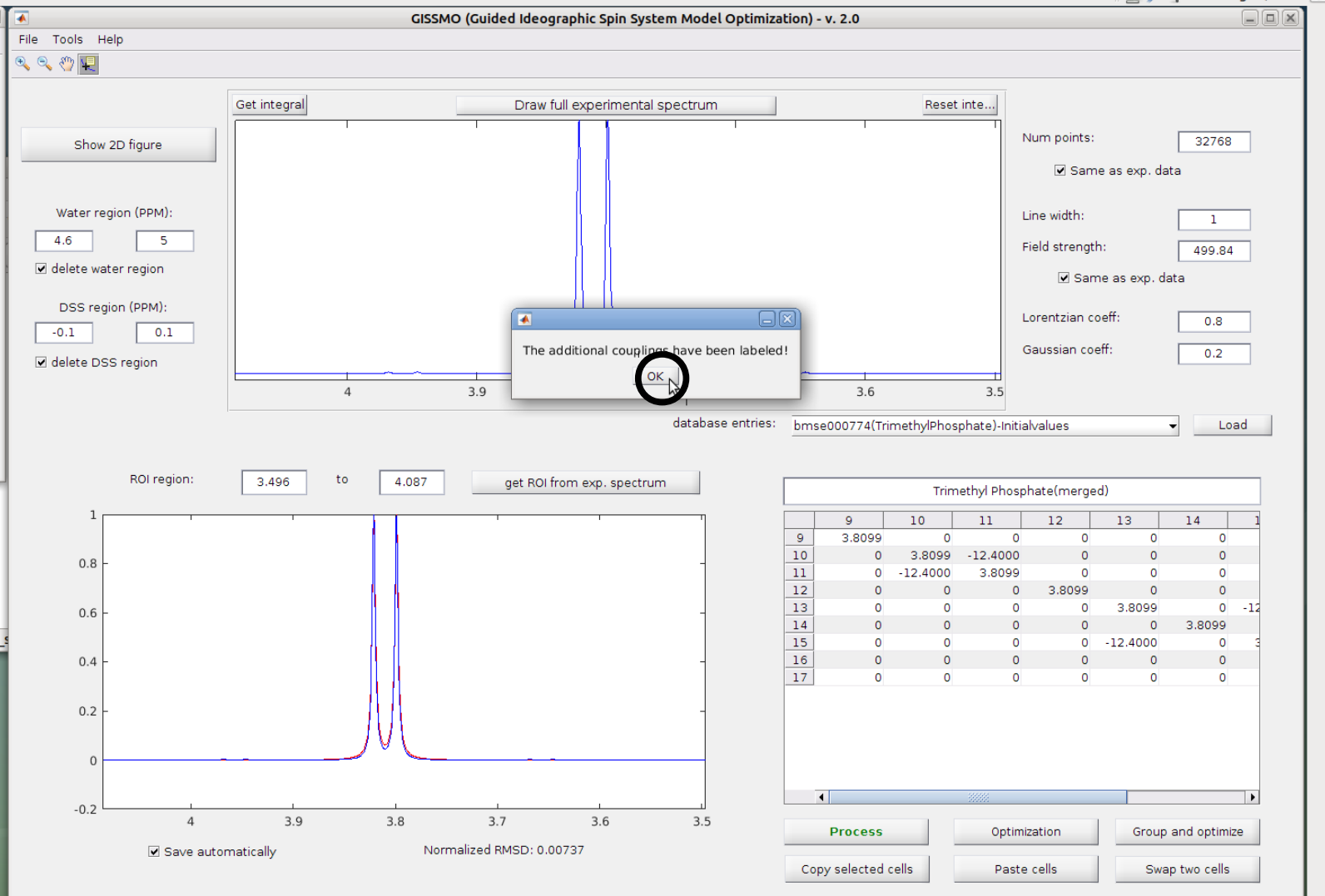


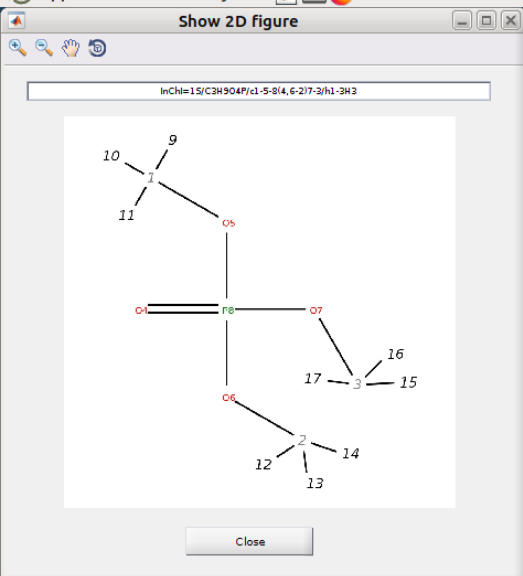


Network

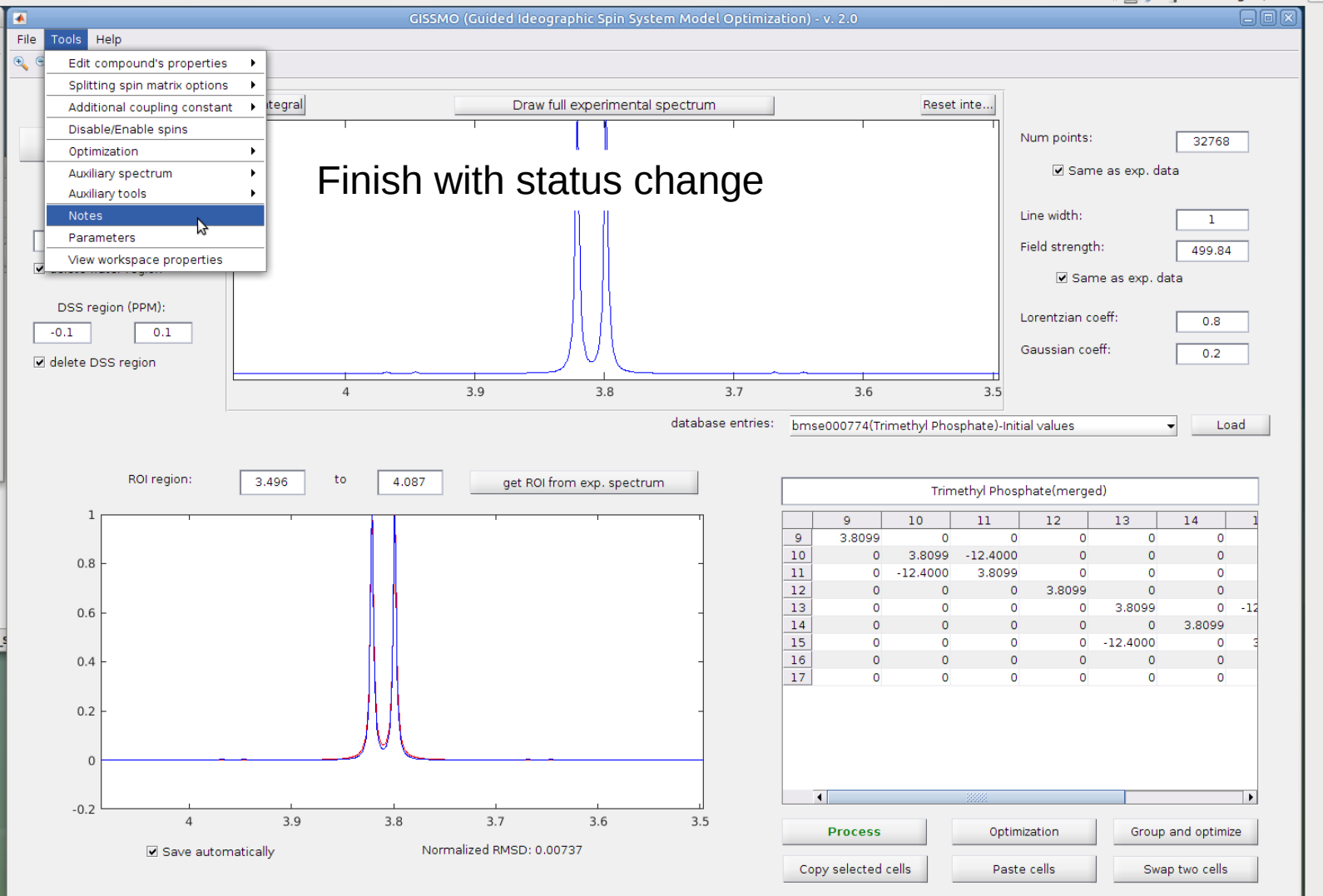
Brow...

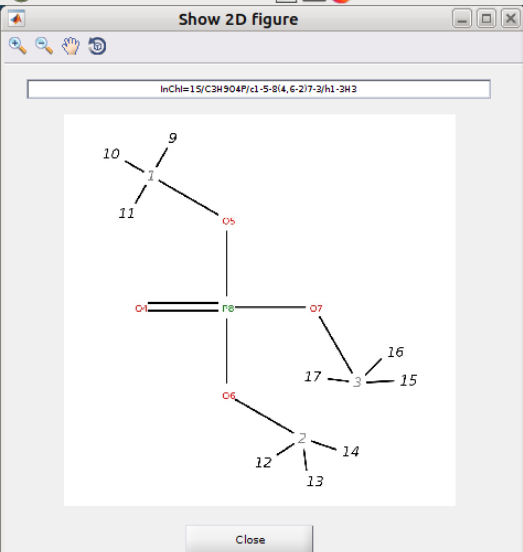
\*spin\_s





Network  
Brow...





Network  
Brow...

GISSMO

File Tools Help

Get integral

Show 2D figure

Water region (PPM):  
4.6 5  
☒ delete water region

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

Notes

Status:  
Initial values

Notes:  
Non-hydrogen additional coupling:  
spin name(s): "9,10,11,12,13,14,15,16,17", coupling of  
"11.114038" with "P8"

Additional coupling  
labeling added to notes

Apply Cancel

Reset inte...

Num points: 32768  
☒ Same as exp. data

Line width: 1  
Field strength: 499.84  
☒ Same as exp. data

Lorentzian coeff: 0.8  
Gaussian coeff: 0.2

database entries: bmse000774(Trimethyl Phosphate)-Initial values Load

ROI region: 3.496 to 4.087 get ROI from exp. spectrum

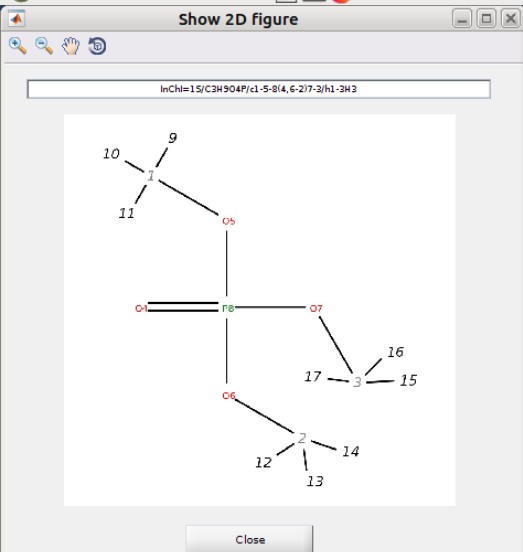
Save automatically

Trimethyl Phosphate(merged)

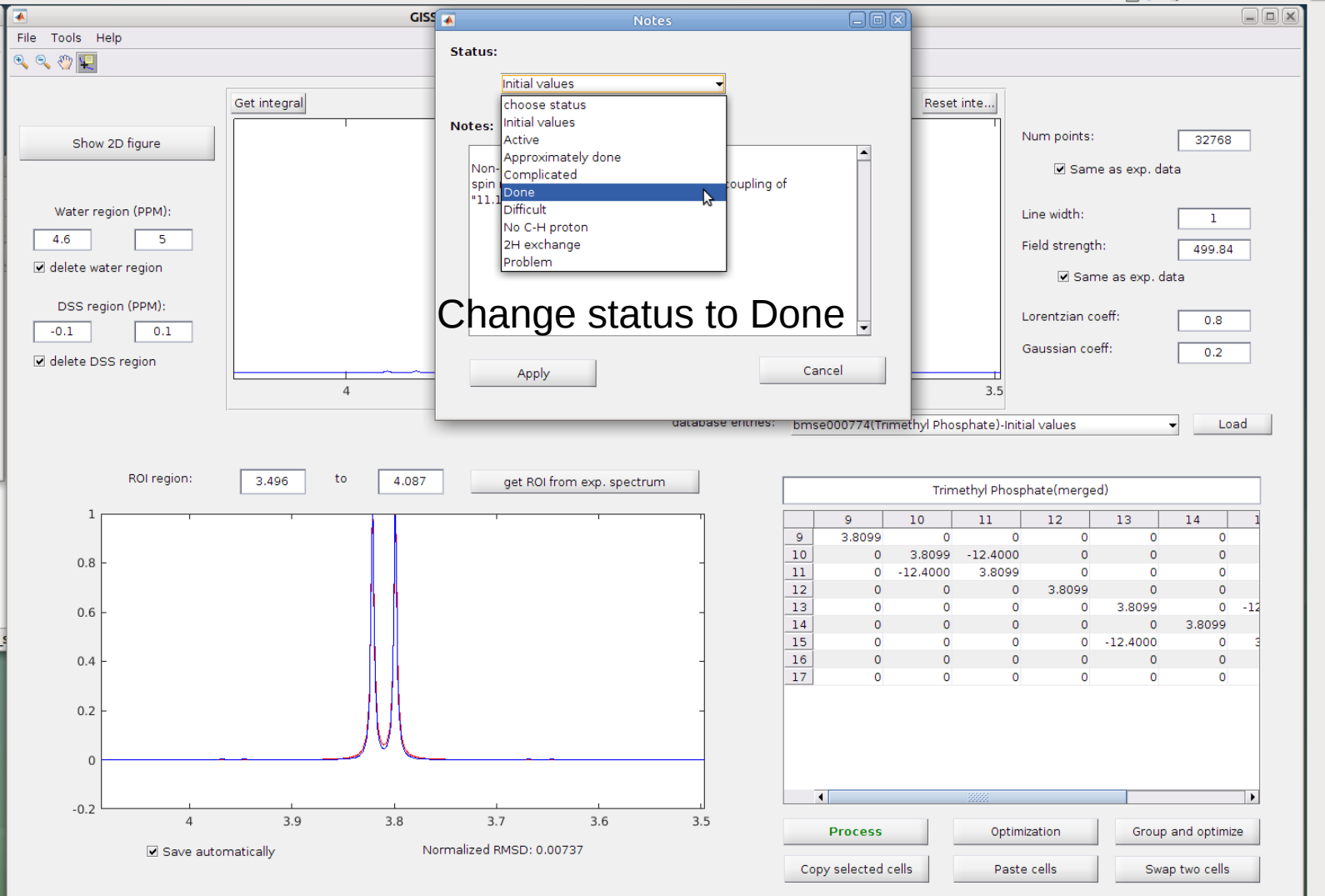
	9	10	11	12	13	14	15	16	17
9	3.8099	0	0	0	0	0	0	0	0
10	0	3.8099	-12.4000	0	0	0	0	0	0
11	0	-12.4000	3.8099	0	0	0	0	0	0
12	0	0	0	3.8099	0	0	0	0	0
13	0	0	0	0	3.8099	0	-12.4000	0	0
14	0	0	0	0	0	3.8099	0	0	0
15	0	0	0	0	-12.4000	0	0	0	0
16	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0

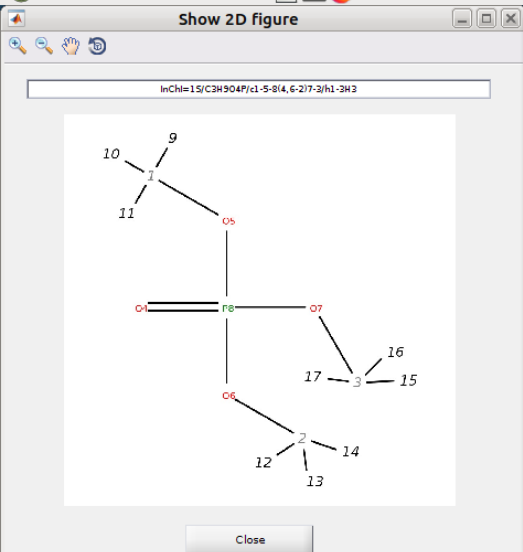
Process Optimization Group and optimize  
Copy selected cells Paste cells Swap two cells





Network  
Brow...





Network  
Brow...

GISSMO

File Tools Help

Get integral

Show 2D figure

Water region (PPM):  
4.6 5  
☒ delete water region

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

Notes

Status: Done

Notes:  
Non-hydrogen additional coupling:  
spin name(s): "9,10,11,12,13,14,15,16,17", coupling of "11.114038" with "P8"

Apply

Cancel

Reset inte...

Num points: 32768  
☒ Same as exp. data

Line width: 1  
Field strength: 499.84  
☒ Same as exp. data

Lorentzian coeff: 0.8  
Gaussian coeff: 0.2

database entries: bmse000774(Trimethyl Phosphate)-Initial values Load

ROI region: 3.496 to 4.087 get ROI from exp. spectrum

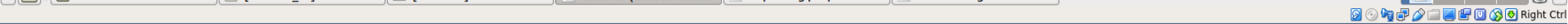
Save automatically

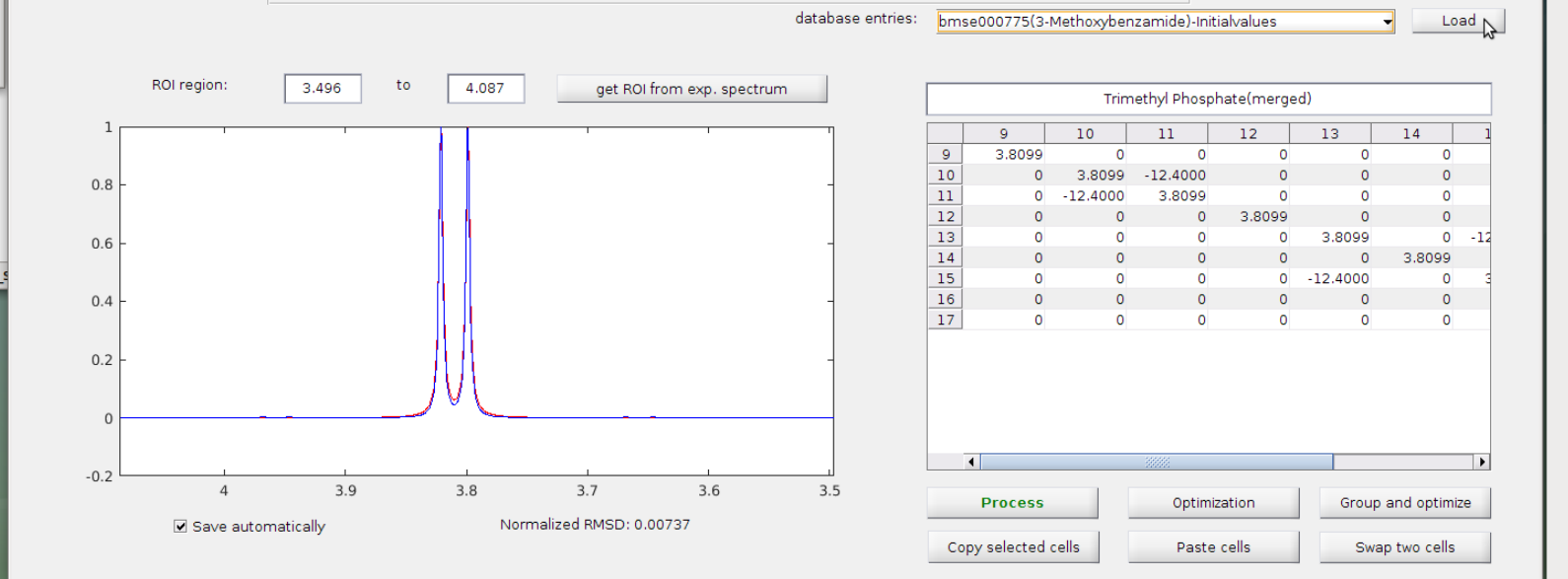
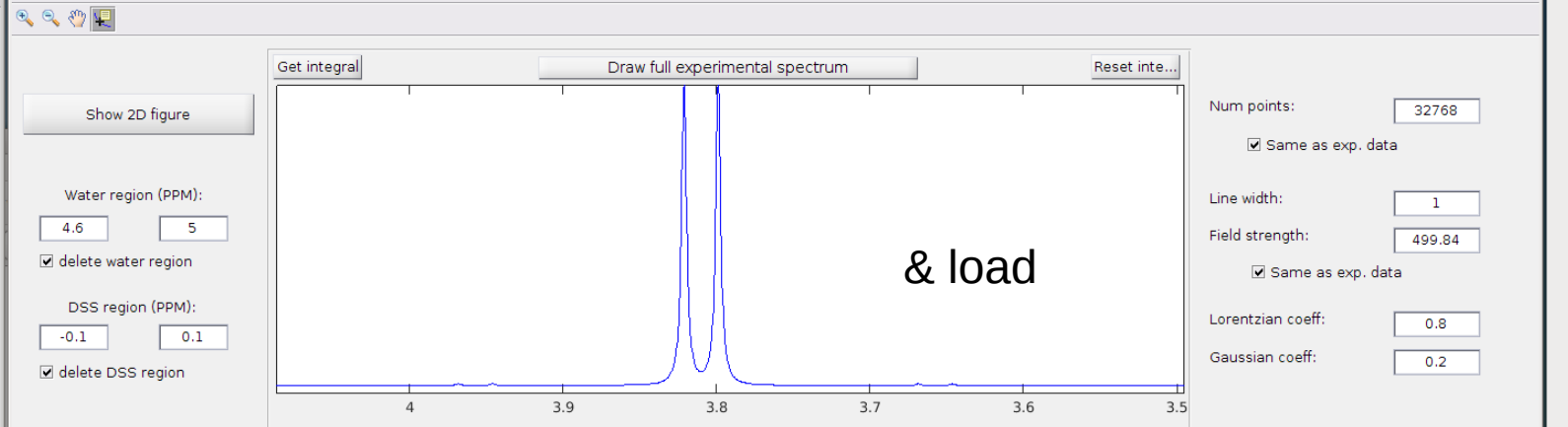
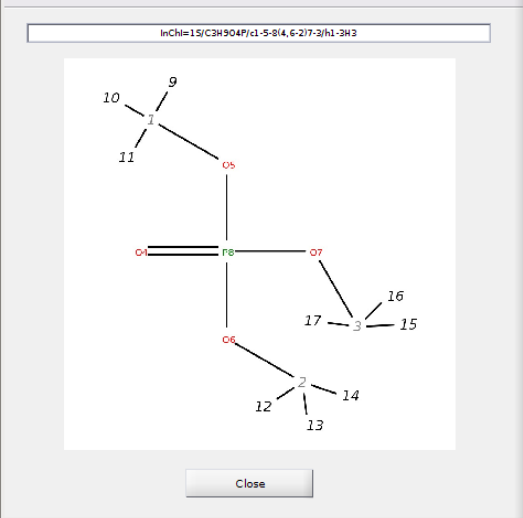
Normalized RMSD: 0.00737

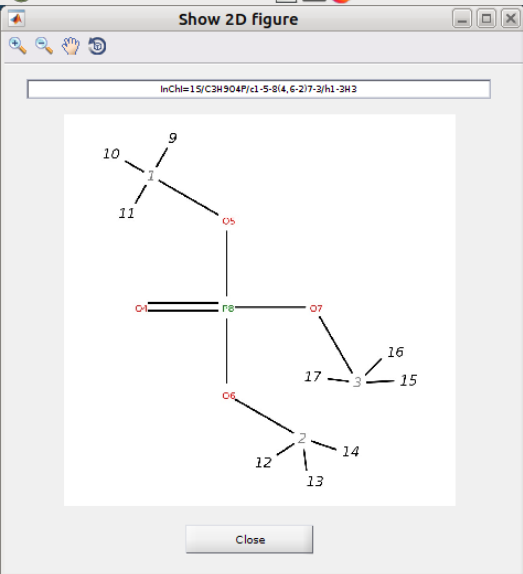
Trimethyl Phosphate(merged)							
	9	10	11	12	13	14	15
9	3.8099	0	0	0	0	0	0
10	0	3.8099	-12.4000	0	0	0	0
11	0	-12.4000	3.8099	0	0	0	0
12	0	0	0	3.8099	0	0	0
13	0	0	0	0	3.8099	0	-12.4000
14	0	0	0	0	0	3.8099	0
15	0	0	0	0	-12.4000	0	3.8099
16	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0

Process Optimization Group and optimize

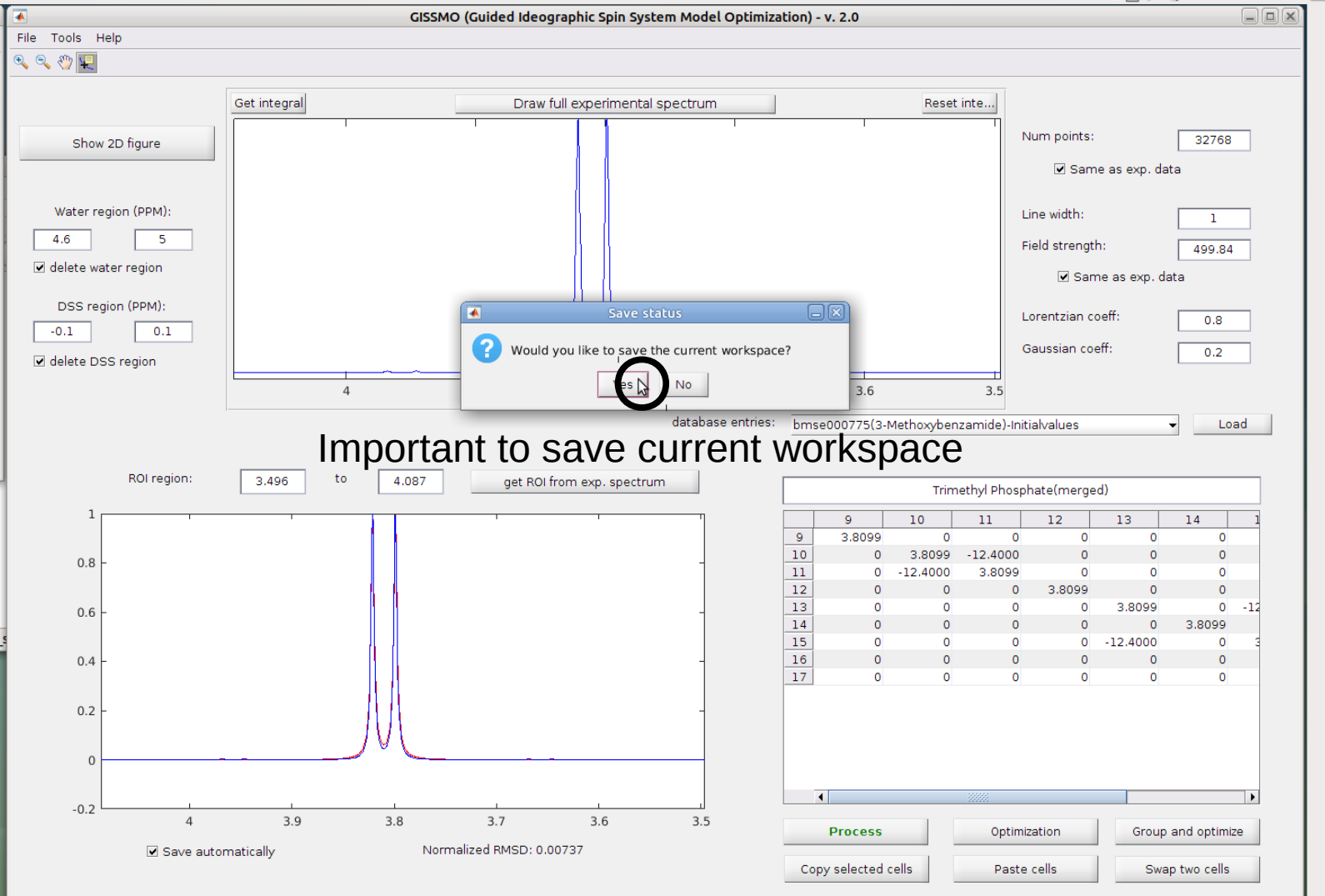
Copy selected cells Paste cells Swap two cells

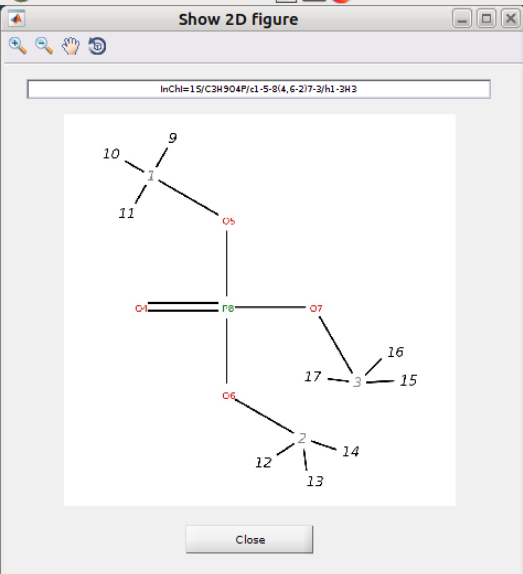






Network  
Brow...





Network  
Brow...  
\*spin\_s

