

**Spectral Similarity Search based on  
20,000,000 Structures  
downloadable from the INTERNET  
using CSEARCH - Technology**

**Description of Request**

Please cite this service as:

W. Robien; <http://c13nmr.at/similar/eval.php>

**Automatic Resubmit:**

**Multiplicity omitted**

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:08

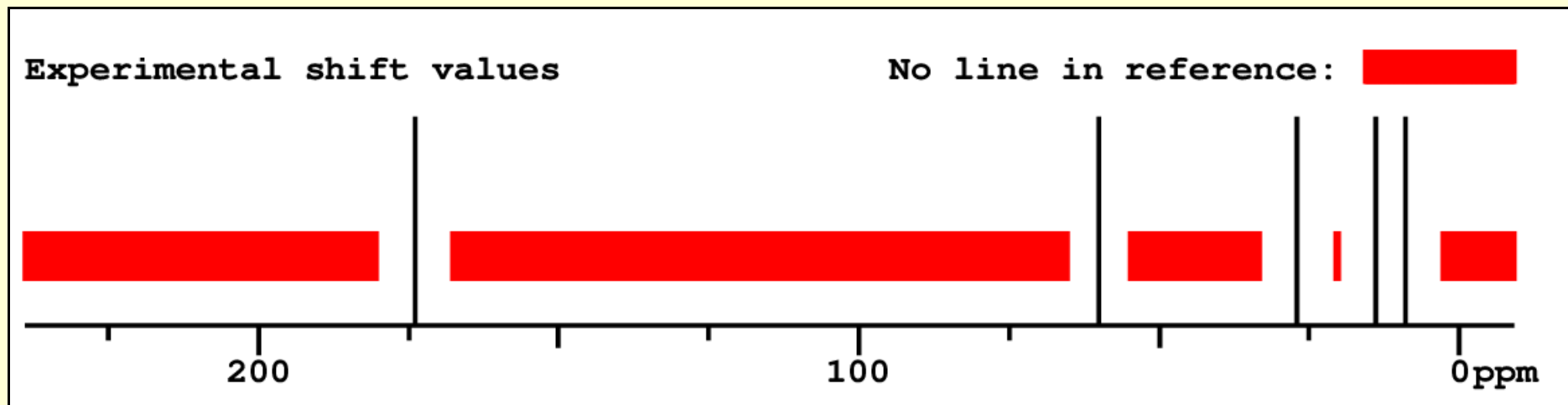
This page will be kept for 30 days here

<b>Name of Project:</b>	Test1
<b>Comment:</b>	Dereplication-engine
<b>Name of Compound:</b>	Propionic_acid,ethylester 400MHz

### Summary of Supplied Data

Peaklist given - consists of 5 Lines				
Line number	Chemical Shift (ppm)	Multiplicity	Hydrogens	Deviation (ppm)
1	174.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00
2	60.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	2.50
3	27.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00

4	14.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00
5	9.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00



<b>Additional Constraints given</b>	
Any range more than 2*deviation (ppm) away from a query shiftvalue remains without line(s) in reference compounds	
Minimum number of signals in reference compounds:	3
Maximum number of signals in reference compounds:	7
Constraint from molecular weight already applied during search	

<b>Lower limit for molecular weight:</b>	<b>85.00</b>
<b>Upper limit for molecular weight:</b>	<b>120.00</b>
<b>N</b>	<b>Element must be absent</b>
<b>O</b>	<b>Element must be present</b>
<b>P</b>	<b>Element must be absent</b>
<b>S</b>	<b>Element must be absent</b>
<b>F</b>	<b>Element must be absent</b>
<b>Cl</b>	<b>Element must be absent</b>
<b>Br</b>	<b>Element must be absent</b>
<b>I</b>	<b>Element must be absent</b>
<b>other</b>	<b>Element must be absent</b>

#### Elemental Composition of Reference Structures

<b>Total number of reference compounds:</b>	<b>20,000,000</b>
<b>Compounds containing: N</b>	<b>19,179,234</b>
<b>Compounds containing: O</b>	<b>17,609,640</b>
<b>Compounds containing: P</b>	<b>14,598</b>
<b>Compounds containing: S</b>	<b>4,210,115</b>
<b>Compounds containing: F</b>	<b>3,311,410</b>
<b>Compounds containing: Cl</b>	<b>1,528,131</b>
<b>Compounds containing: Br</b>	<b>662,509</b>
<b>Compounds containing: I</b>	<b>50,080</b>
<b>Compounds containing: other</b>	<b>60,083</b>

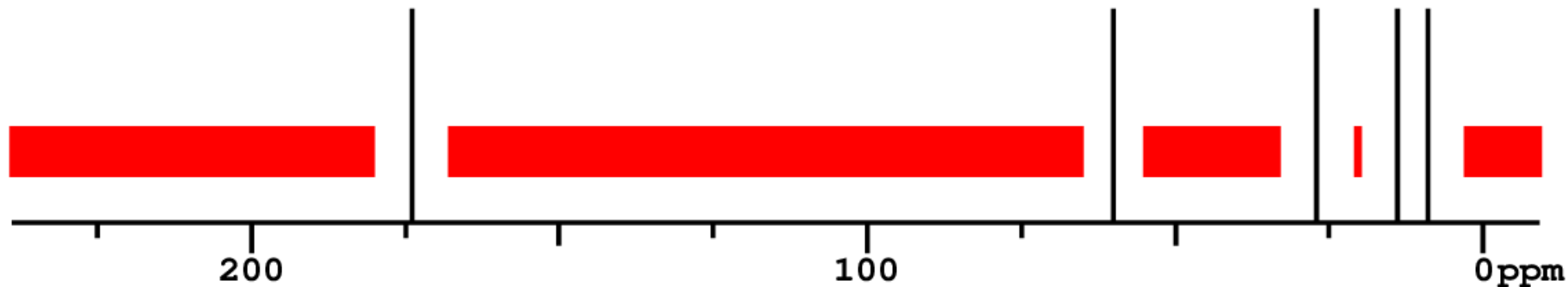
Available entries at each Screening-Step

<b>Total number of entries:</b>	<b>20,000,000</b>
<b>Applying requested elemental composition:</b>	<b>510,515 entries remain</b>
<b>Applying requested number of signals:</b>	<b>16,134 entries remain</b>

<b>Entries per line found out of 16,134 compounds</b>					
<b>Line number</b>	<b>Chemical Shift (ppm)</b>	<b>Multiplicity</b>	<b>Deviation (ppm)</b>	<b>Entries found</b>	<b>Evaluation result</b>
<b>1</b>	<b>174.00</b>	<b>?</b>	<b>3.00</b>	<b>1,572</b>	<b>Impurity ?</b>
<b>2</b>	<b>60.00</b>	<b>?</b>	<b>2.50</b>	<b>2,891</b>	<b>Unspecific line</b>
<b>3</b>	<b>27.00</b>	<b>?</b>	<b>3.00</b>	<b>5,086</b>	<b>Unspecific line</b>
<b>4</b>	<b>14.00</b>	<b>?</b>	<b>3.00</b>	<b>3,842</b>	<b>Unspecific line</b>
<b>5</b>	<b>9.00</b>	<b>?</b>	<b>3.00</b>	<b>2,625</b>	<b>Unspecific line</b>

Experimental shift values

No line in reference: 



Number of coincident lines versus number of entries

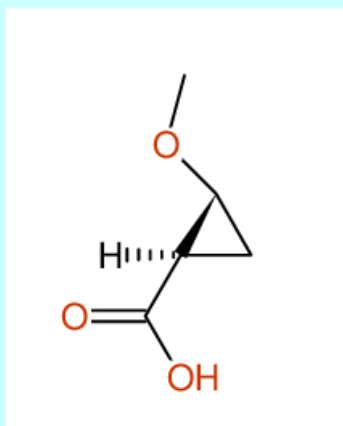
Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	7	Selected for detailed analysis
4	131	Selected for detailed analysis
3	798	Selected for detailed analysis
2	3,293	Selected for detailed analysis
1	6,477	

Best 13 Proposals shown for Compound: Propionic\_acid,ethylester::400MHz

3.49 -  
3.49ppm

1x found

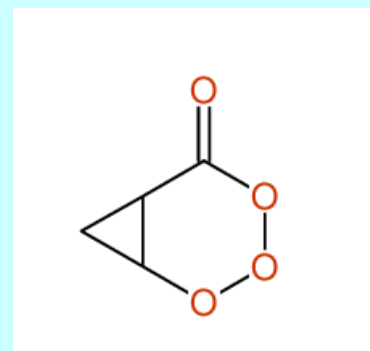
[LAWCUGGFTNCKX](#)



5.25 -  
5.25ppm

1x found

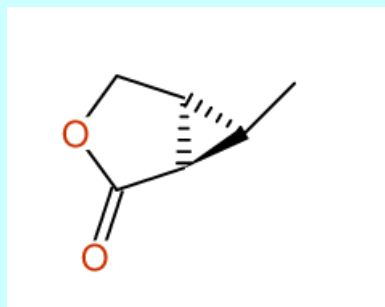
[CRVCBHWPBDCDX](#)



6.04 -  
6.04ppm

1x found

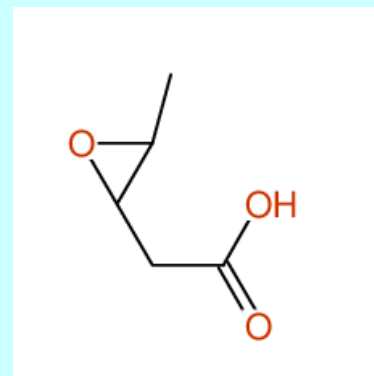
[ODZSNSOKRZBPDY](#)



6.82 -  
6.90ppm

2x found

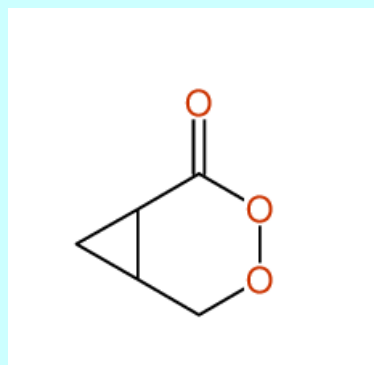
[GQIWAJFJHVXXBY](#)



8.26 -  
8.26ppm

1x found

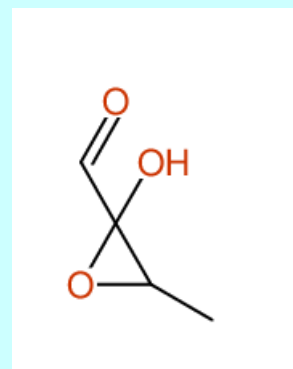
[LSONYXQSJHZPCV](#)



8.43 -  
8.43ppm

1x found

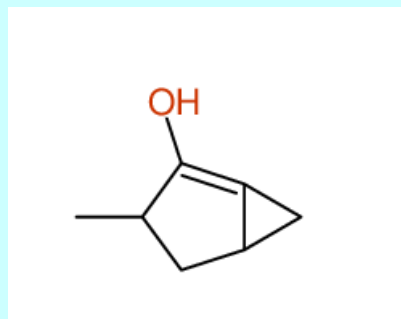
[GTUSACQZTIXZFX](#)



8.65 -  
8.65ppm

1x found

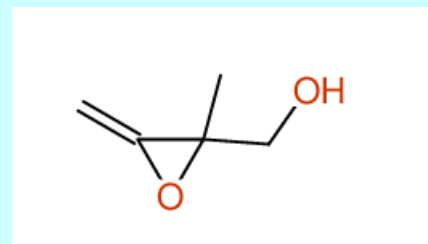
[WQZCEYRBPLRVQT](#)



8.75 -  
8.75ppm

1x found

[QIJHBLJRPKBWEU](#)

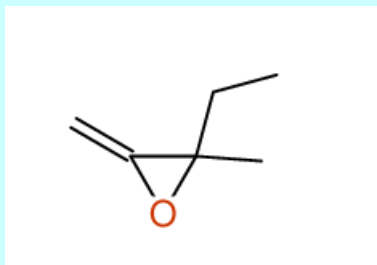




9.45 -  
9.45ppm

1x found

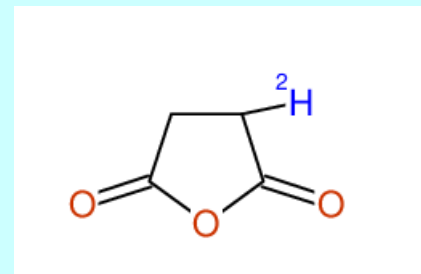
[HUZIABIIKFXMOH](#)



9.47 -  
9.47ppm

1x found

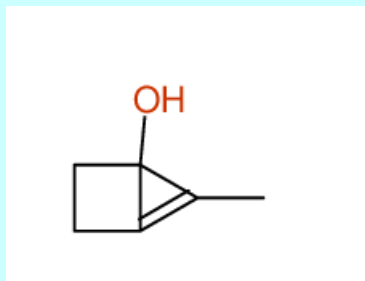
[RINCXYDBBGEEQ](#)



9.51 -  
9.51ppm

1x found

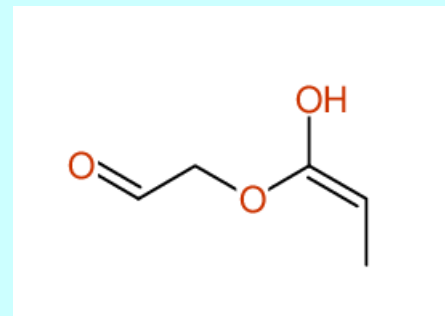
[WPNREIWMCOZWLX](#)



9.51 -  
9.51ppm

1x found

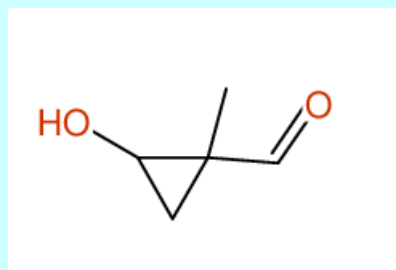
[LNDNUFLSISIDOD](#)



9.56 -  
9.56ppm

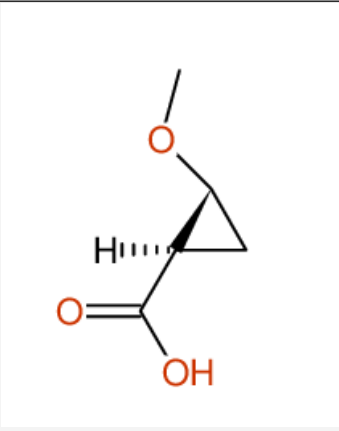
1x found

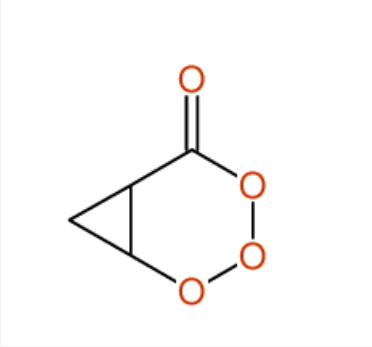
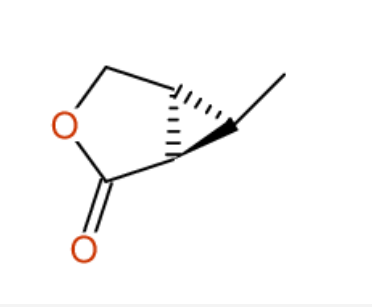

[ZOUPILOGYBSRVKU](#)


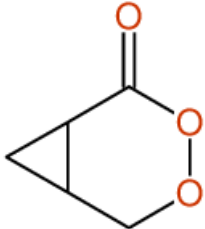
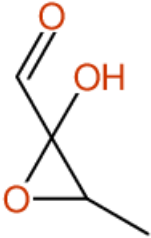


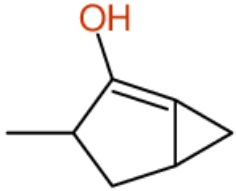
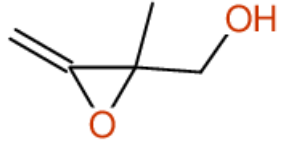
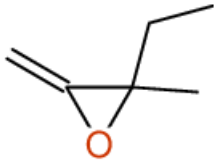
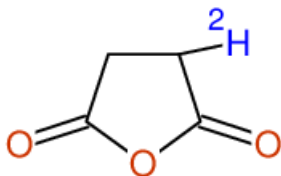

4,229 [Structure proposals](#) found for your C-NMR Spectrum

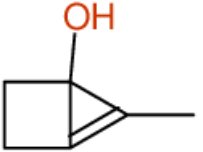
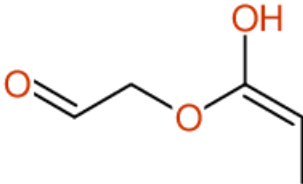

438 Entries will be shown because of your selection of additional constraints

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1  3.49 <a href="#">Details</a>	 <p>Chemical structure diagram showing a cyclopropane ring with a methoxy group (OCH<sub>3</sub>) and a methyl group attached to one carbon, and an aldehyde group (CHO) attached to another carbon. The hydrogen on the ring is shown with a dashed bond.</p>	C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> MWT = 116.055	Proposal #1 Structure-ID: 18,262,813 <a href="#">LAWCUGGFTNCKX-SRBOSORUBI</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #2</p> <p>5.25</p> <p><a href="#">Details</a></p>		<p><math>C_4H_4O_4</math></p> <p>MWT = 116.044</p>	<p>Proposal #2</p> <p>Structure-ID: 627,828</p> <p><a href="#">CRVCBHWPBDXCDX-UHFFFAOYAF</a></p>	
<p>Proposal #3</p> <p>6.04</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_8O_2</math></p> <p>MWT = 112.066</p>	<p>Proposal #3</p> <p>Structure-ID: 18,263,141</p> <p><a href="#">ODZSNSOKRZBPDY-LJJLCWGRBL</a></p>	
<p>Proposal #4</p> <p>6.82</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_8O_3</math></p> <p>MWT = 116.055</p>	<p>Proposal #4</p> <p>Structure-ID: 3,277,468</p> <p><a href="#">GQIWAJFJHVXXBY-QWWZWVQMBW</a></p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #5</p> <p>6.90</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_8O_3</math></p> <p>MWT = 116.055</p>	<p>Proposal #5</p> <p>Structure-ID: 3,277,470</p> <p><a href="#">GQIWAJFJHVXXBY-IUYQGCFVBG</a></p>	
<p>Proposal #6</p> <p>8.26</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_6O_3</math></p> <p>MWT = 114.055</p>	<p>Proposal #6</p> <p>Structure-ID: 627,804</p> <p><a href="#">LSONYXQSJHZPCV-UHFFFAOYAP</a></p>	
<p>Proposal #7</p> <p>8.43</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_4H_6O_3</math></p> <p>MWT = 102.044</p>	<p>Proposal #7</p> <p>Structure-ID: 17,071,481</p> <p><a href="#">GTUSACQZTIXZFX-UHFFFAOYAS</a></p>	

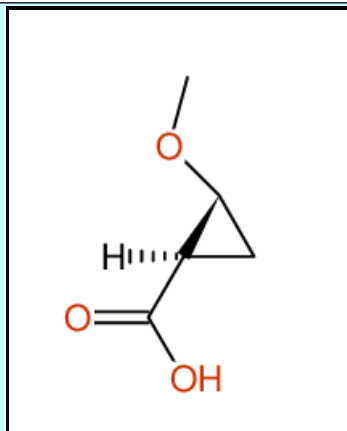
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #8</p> <p>8.65</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_7H_{10}O</math></p> <p>MWT = 110.077</p>	<p>Proposal #8</p> <p>Structure-ID: 654,774</p> <p><a href="#">WQZCEYRBPLRVQT-UHFFFAOYAN</a></p>	
<p>Proposal #9</p> <p>8.75</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_8O_2</math></p> <p>MWT = 100.055</p>	<p>Proposal #9</p> <p>Structure-ID: 17,071,769</p> <p><a href="#">QIJHBLJRPKBWEU-UHFFFAOYAP</a></p>	
<p>Proposal #10</p> <p>9.45</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{10}O</math></p> <p>MWT = 98.066</p>	<p>Proposal #10</p> <p>Structure-ID: 17,071,790</p> <p><a href="#">HUZIABIIKFXMOH-UHFFFAOYAZ</a></p>	
<p>Proposal #11</p> <p>9.47</p> <p><a href="#">Details</a></p>		<p><math>C_4H_4O_3</math></p> <p>MWT = 101.044</p>	<p>Proposal #11</p> <p>Structure-ID: 7,029,234</p> <p><a href="#">RINCXYDBBGOEEQ-MICDWDJOJE</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #12  9.51  <a href="#">Details</a>		$C_6H_{10}O$ MWT = 96.066	Proposal #12 Structure-ID: 16,814,789 <a href="#">WPNREIWMCOZWLX-UHFFFAOYAR</a>	
Proposal #13  9.51  <a href="#">Details</a>  Different pattern		$C_5H_8O_3$ MWT = 116.055	Proposal #13 Structure-ID: 760,473 <a href="#">LNDNUFLSISIDOD-UHFFFAOYAZ</a>	
Proposal #14  9.56  <a href="#">Details</a>  Different pattern		$C_5H_8O_2$ MWT = 100.055	Proposal #14 Structure-ID: 17,071,377 <a href="#">ZOUPILOGYBSRVKU-UHFFFAOYAV</a>	

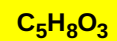
## Detailed Analysis

### Structure Proposal #1

Structure	Similarity Measure



Deviation = 3.49 ppm  
Similarity = 80 %



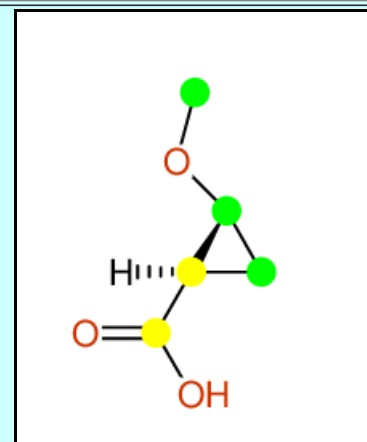
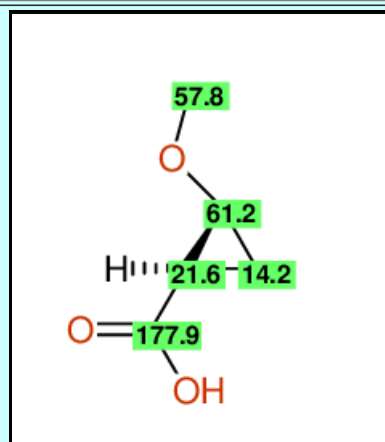
MWT = 116.06

Search Web for this  
structure:

[LAWCUGGETNCKX](#)

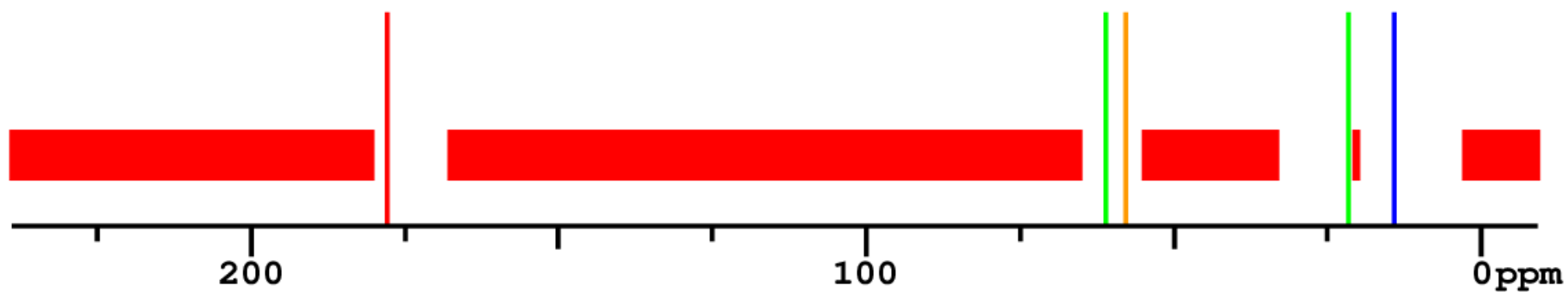
Predicted Chemical  
Shiftvalues

Matching Map



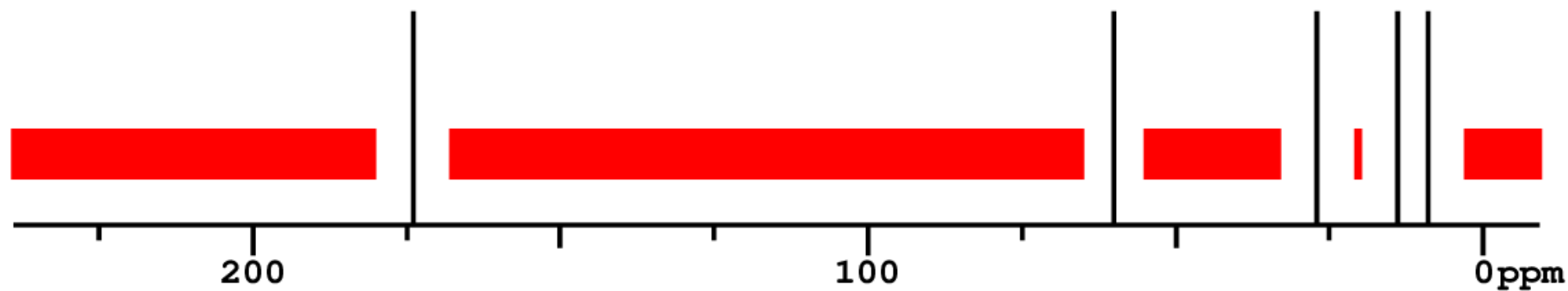
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

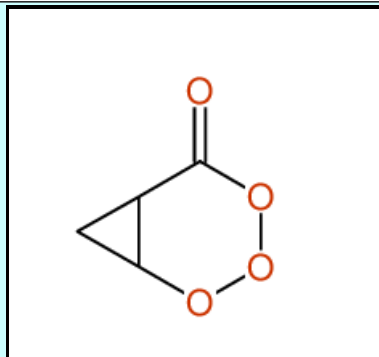


[Back to Complete Result](#)

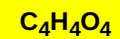
### Structure Proposal #2

Structure	Similarity Measure
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Deviation = 5.25 ppm  
Similarity = 88 %

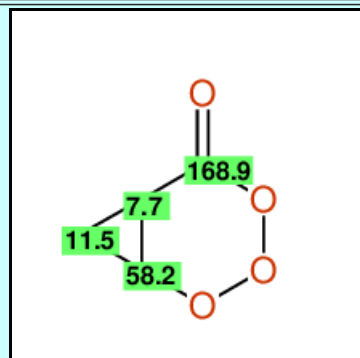


MWT = 116.04

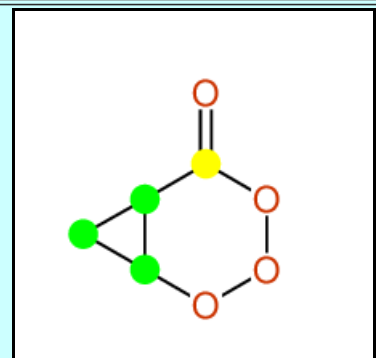
Search Web for this  
structure:

[CRVCBHWPBDXCDX](#)

Predicted Chemical  
Shiftvalues

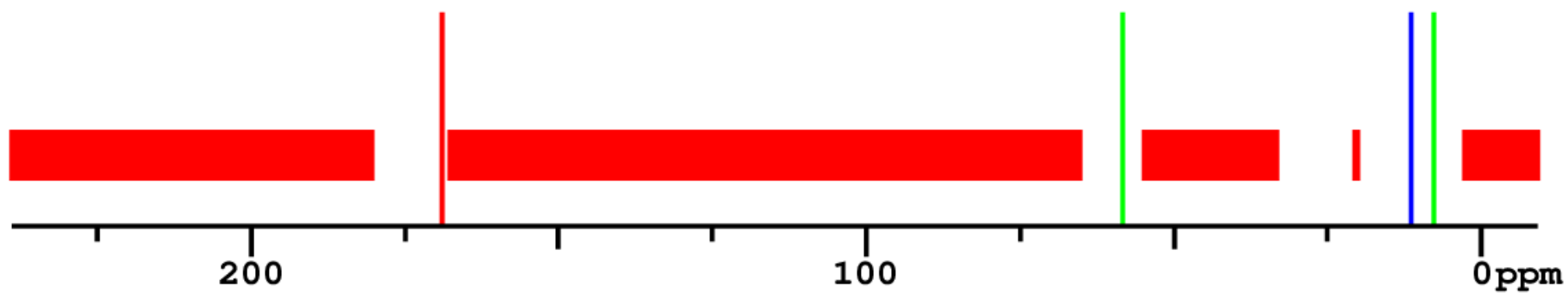


Matching Map



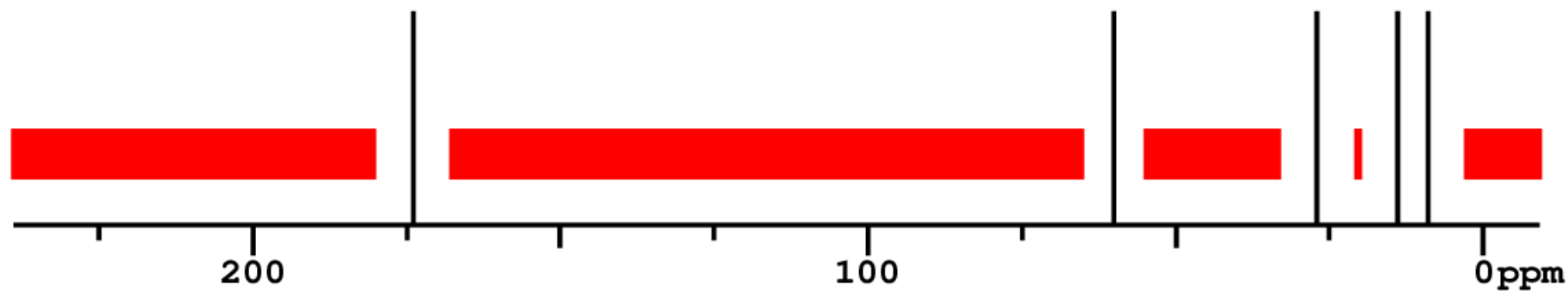
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

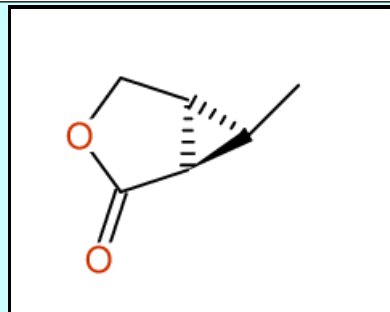
No line in reference: [red bar]



[Back to Complete Result](#)

### Structure Proposal #3

Structure	Similarity Measure
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Deviation = 6.04 ppm  
Similarity = 60 %  
(Different pattern)

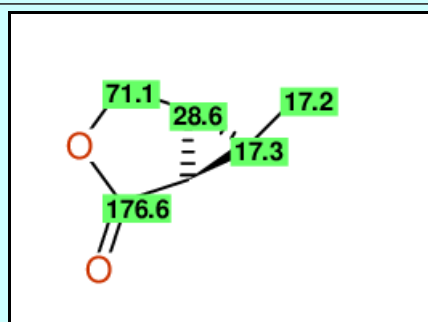


MWT = 112.07

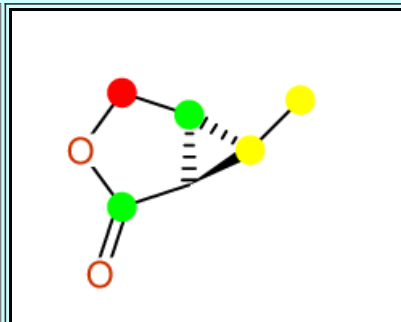
Search Web for this structure:

[ODZSNSOKRZBPDY](#)

Predicted Chemical  
Shiftvalues

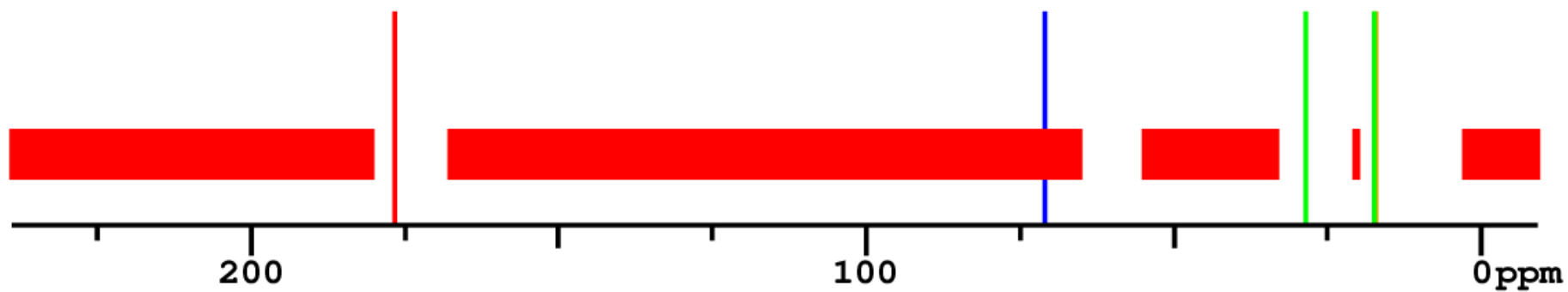


Matching Map



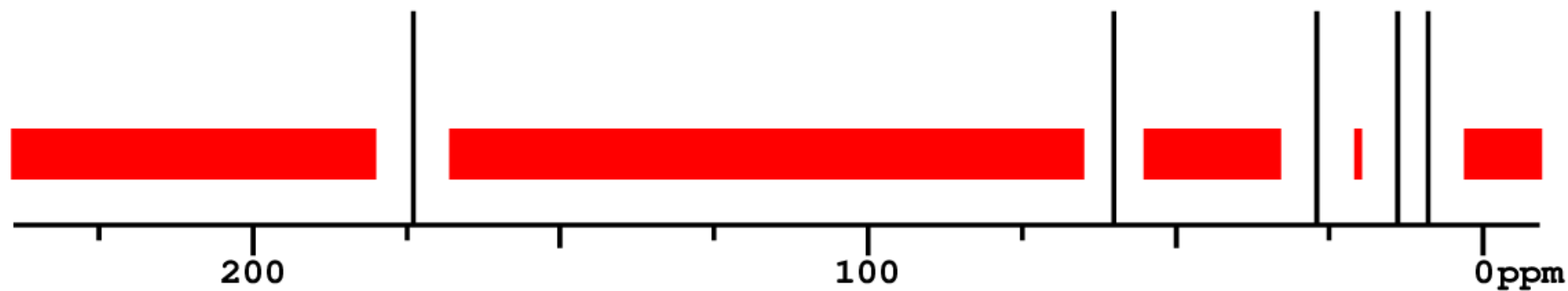
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

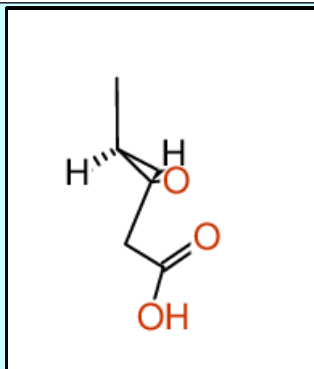
No line in reference: [red bar]



[Back to Complete Result](#)

#### Structure Proposal #4

Structure	Similarity Measure
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Deviation = 6.82 ppm  
 Similarity = 50 %  
 (Different pattern)



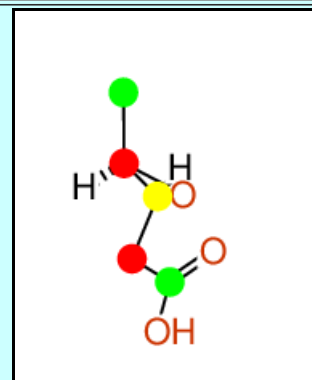
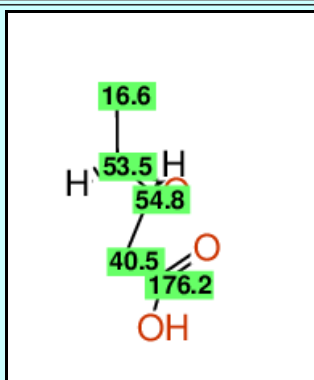
MWT = 116.06

Search Web for this structure:

[GQIWAJFJHVXXBY](https://www.google.com/search?q=GQIWAJFJHVXXBY)

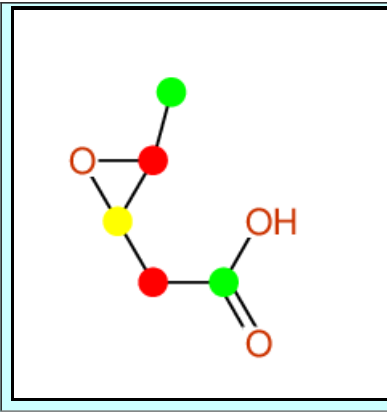
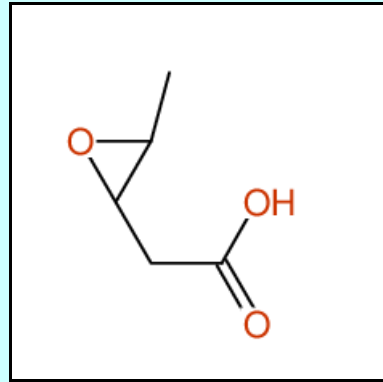
Predicted Chemical Shiftvalues

Matching Map



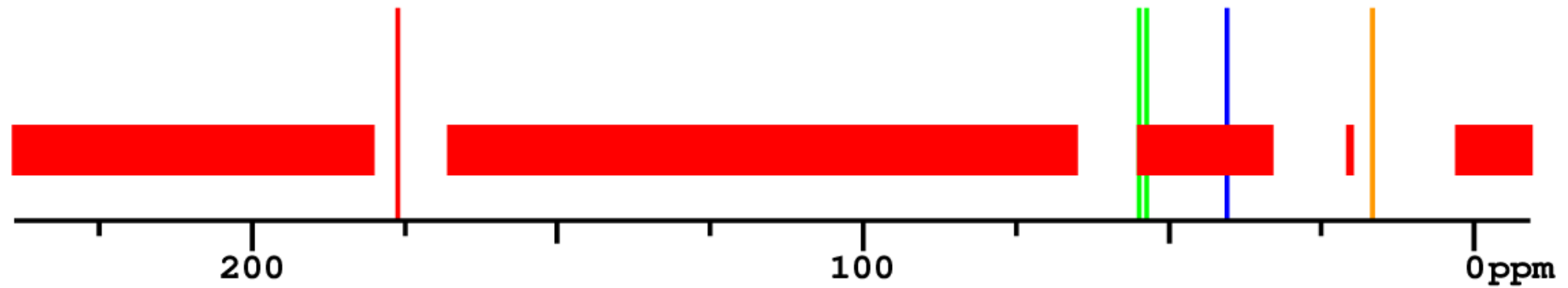
2D Structure Representation

2D Matching Map



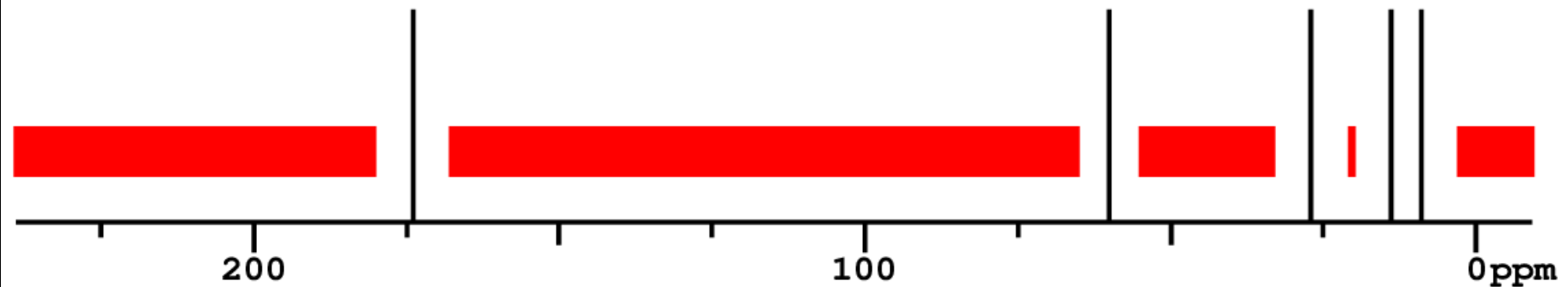
Predicted shift values

Signal multiplicity: S D T Q O E P ?

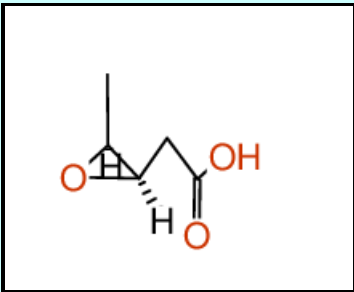
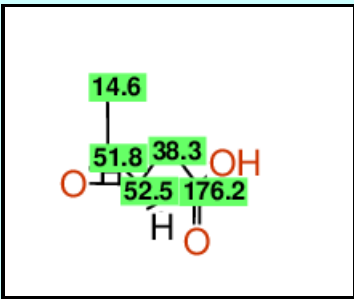
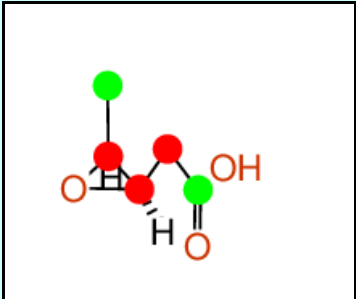


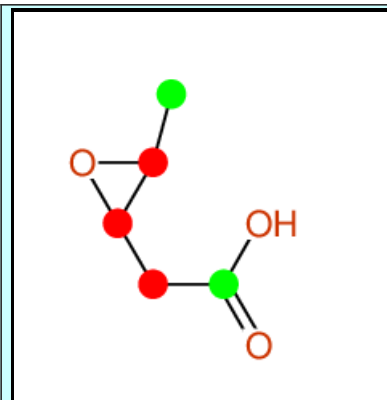
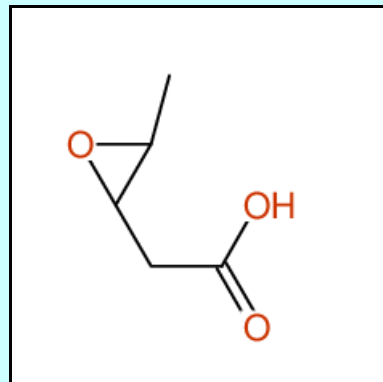
Experimental shift values

No line in reference: 



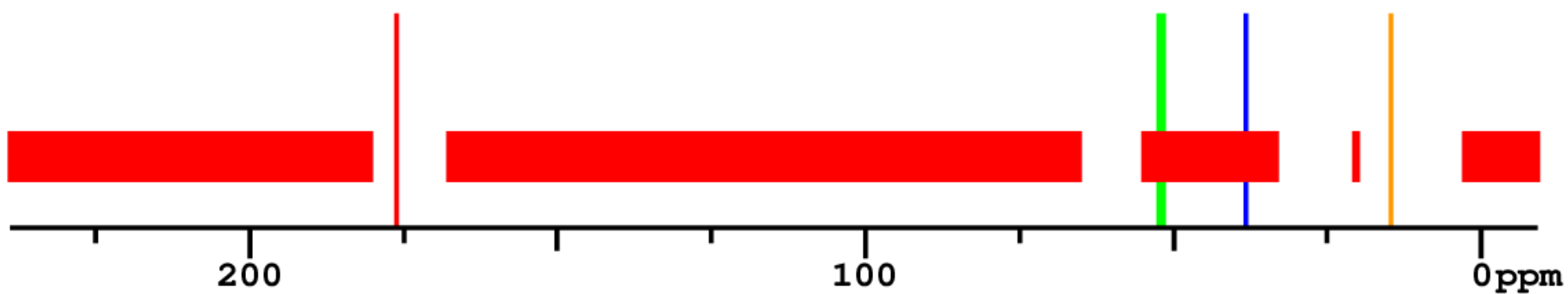
### Structure Proposal #5

Structure	Similarity Measure
	<p>Deviation = 6.90 ppm Similarity = 40 % (Different pattern)</p> <p><math>C_5H_8O_3</math></p> <p>MWT = 116.06</p> <p>Search Web for this structure: <a href="#">GQIWAJFJHVXXBY</a></p>
Predicted Chemical Shiftvalues	Matching Map
	
2D Structure Representation	2D Matching Map



Predicted shift values

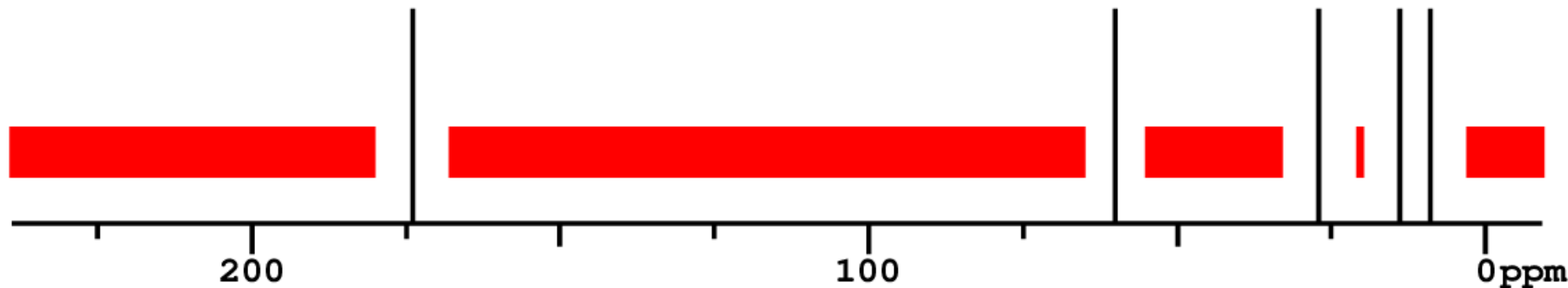
Signal multiplicity: **S****D****T****Q****O****E****P**?





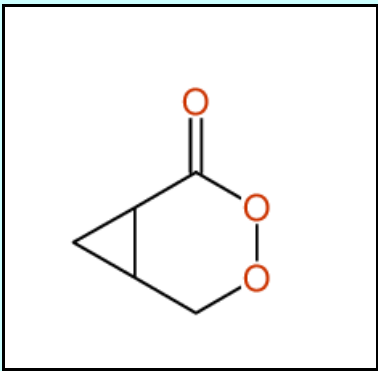
Experimental shift values

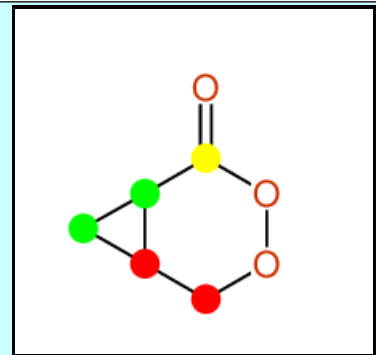
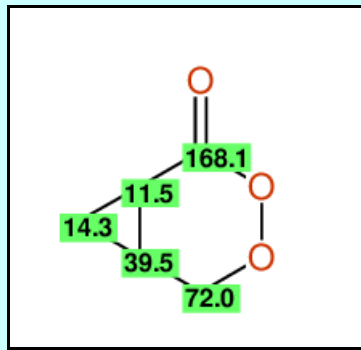
No line in reference: 



[Back to Complete Result](#)

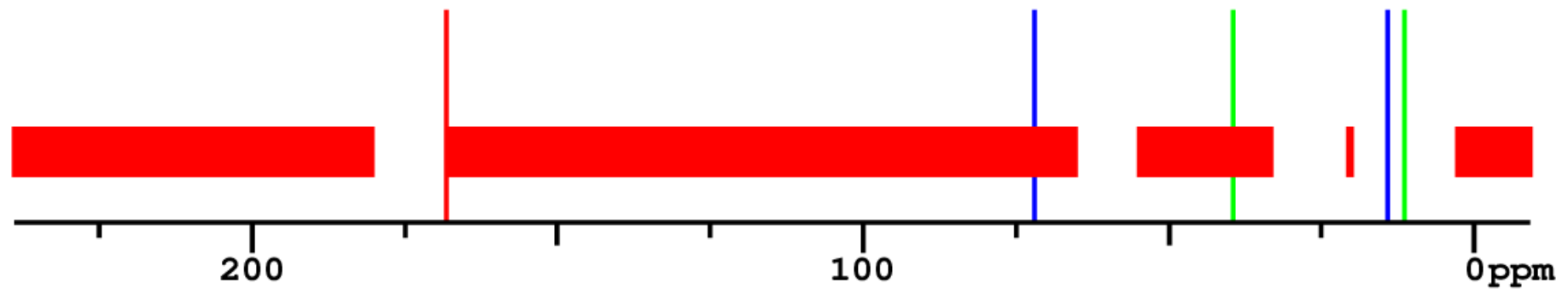
### Structure Proposal #6

Structure	Similarity Measure
	<p>Deviation = 8.26 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_5H_6O_3</math></p> <p>MWT = 114.06</p> <p>Search Web for this structure: <a href="#">LSONYXQSJHZPCV</a></p>
Predicted Chemical Shiftvalues	Matching Map



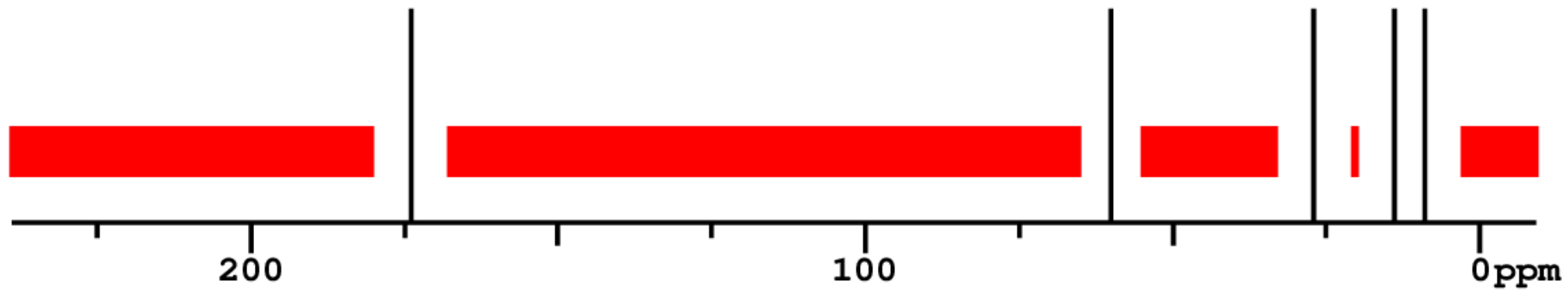
Predicted shift values

Signal multiplicity: S D T Q O E P ?



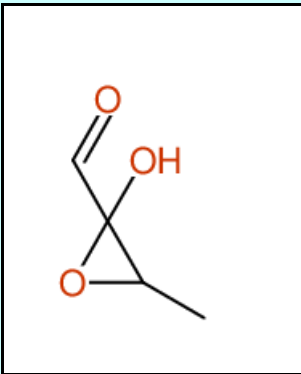
Experimental shift values

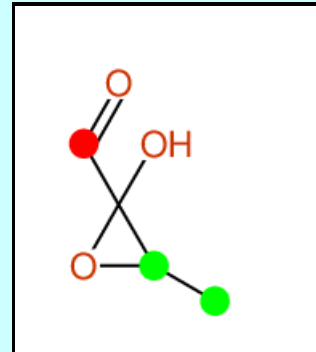
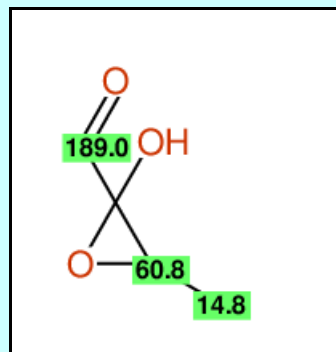
No line in reference: 



[Back to Complete Result](#)

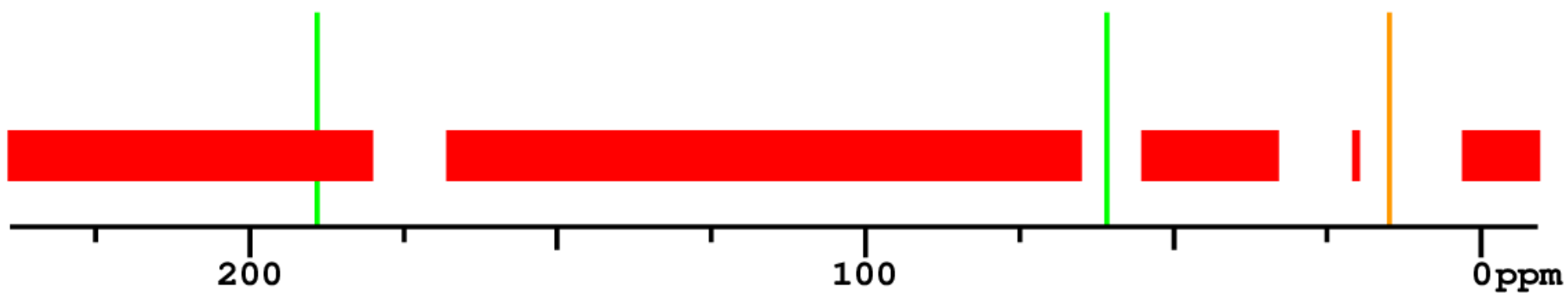
### Structure Proposal #7

Structure	Similarity Measure
	<p>Deviation = 8.43 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_4H_6O_3</math></p> <p>MWT = 102.04</p> <p>Search Web for this structure: <a href="#">GTUSACQZTIXZFX</a></p>
Predicted Chemical Shiftvalues	Matching Map



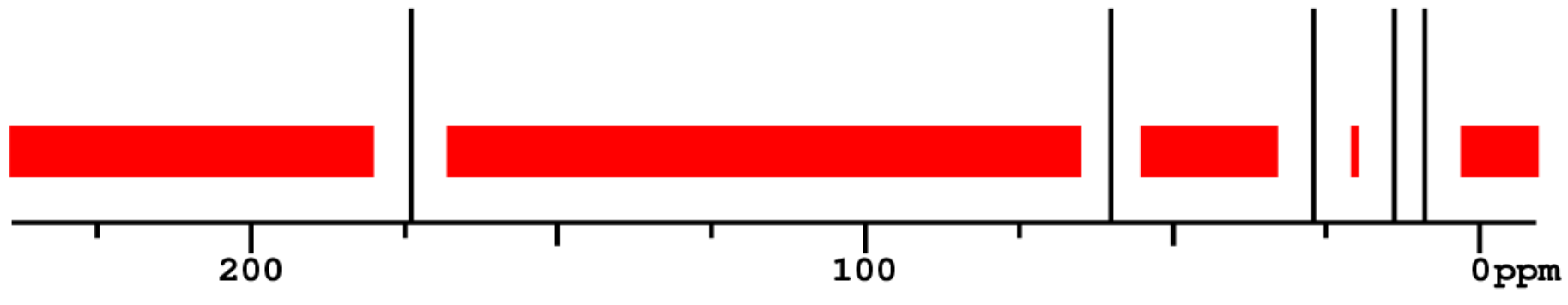
Predicted shift values

Signal multiplicity: S D T Q O E P ?



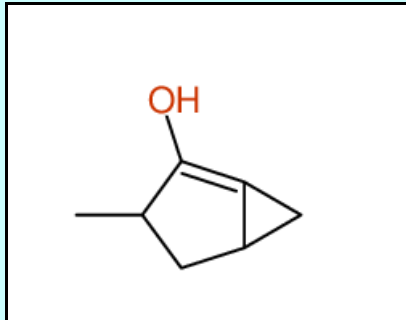
Experimental shift values

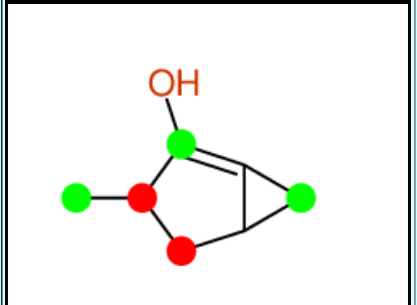
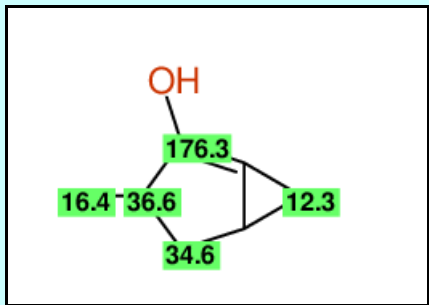
No line in reference: 



[Back to Complete Result](#)

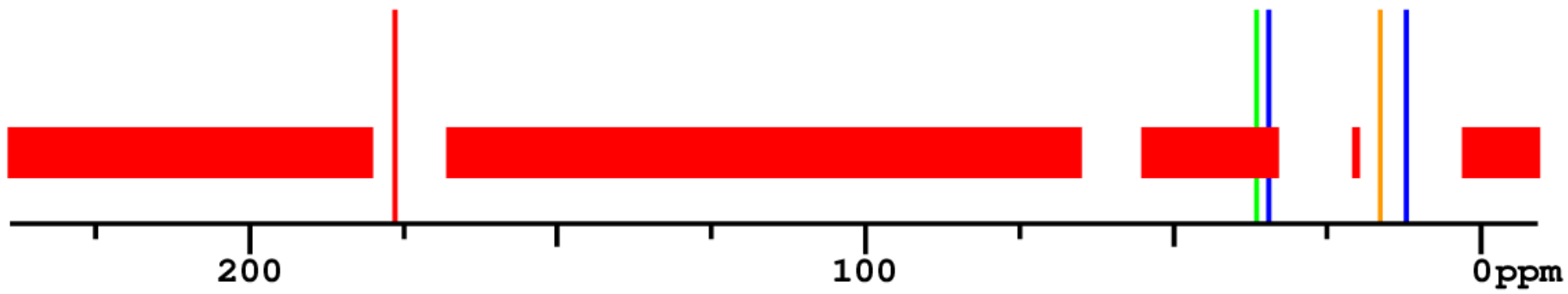
### Structure Proposal #8

Structure	Similarity Measure
	<p>Deviation = 8.65 ppm Similarity = 60 % (Different pattern)</p> <p><math>C_7H_{10}O</math></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">WQZCEYRBPLRVQT</a></p>
Predicted Chemical Shiftvalues	Matching Map



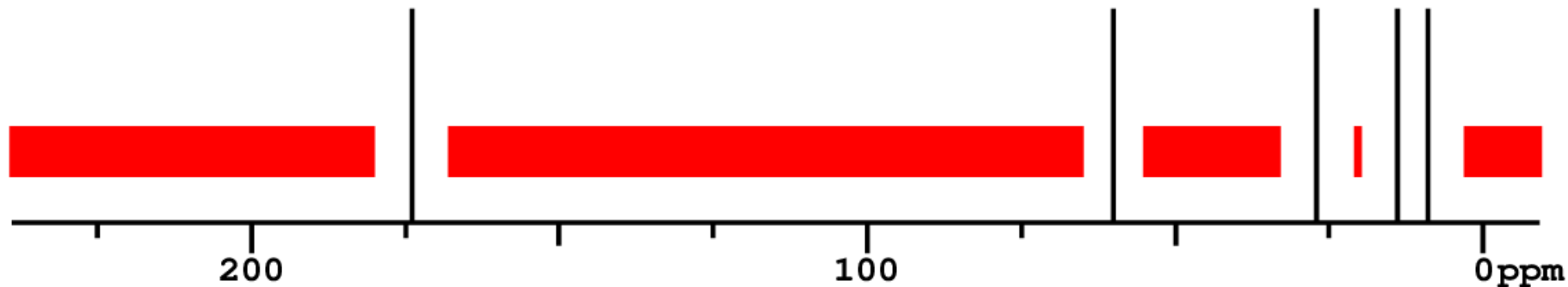
Predicted shift values

Signal multiplicity: S D T Q O E P ?



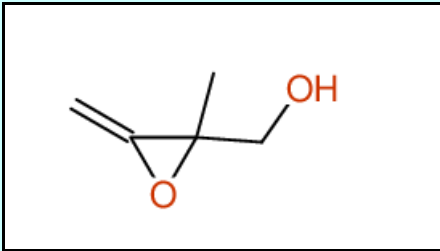
Experimental shift values

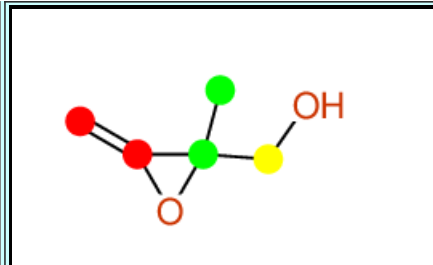
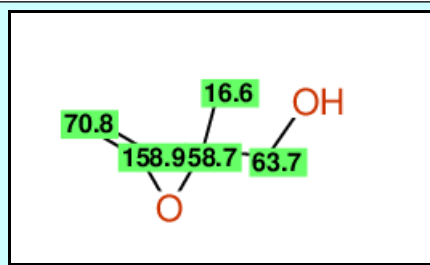
No line in reference: 



[Back to Complete Result](#)

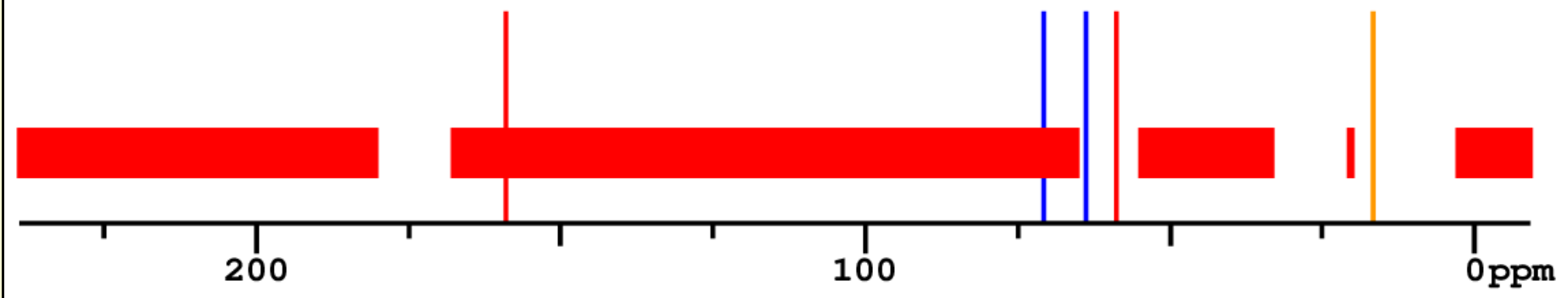
### Structure Proposal #9

Structure	Similarity Measure
	<p>Deviation = 8.75 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_5H_8O_2</math></p> <p>MWT = 100.06</p> <p>Search Web for this structure: <a href="#">QJHBLJRPKBWEU</a></p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

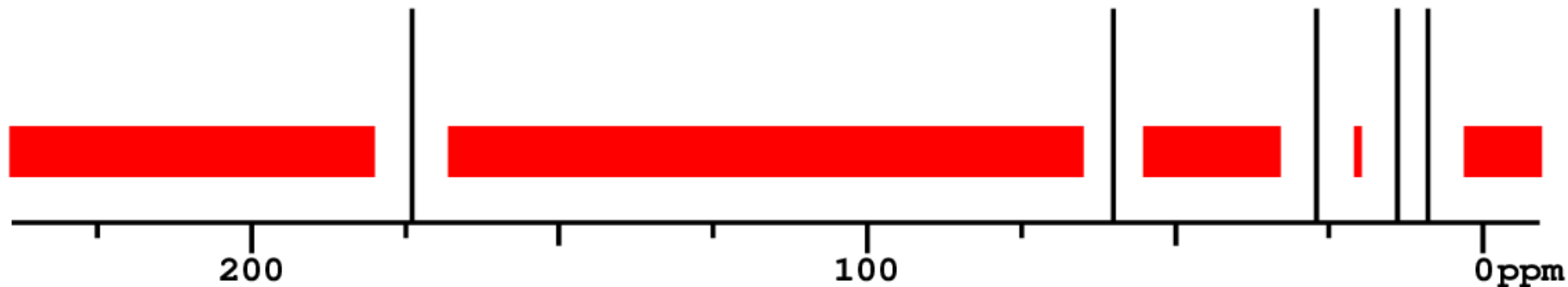
Signal multiplicity: S D T Q O E P ?





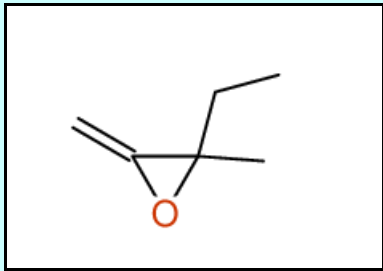
Experimental shift values

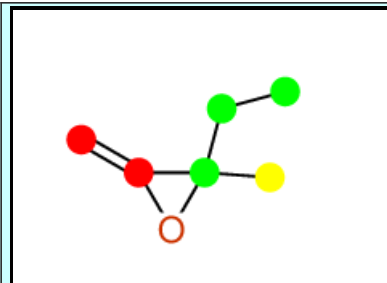
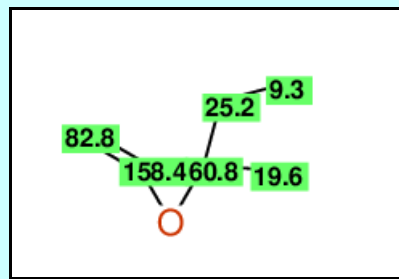
No line in reference: 



[Back to Complete Result](#)

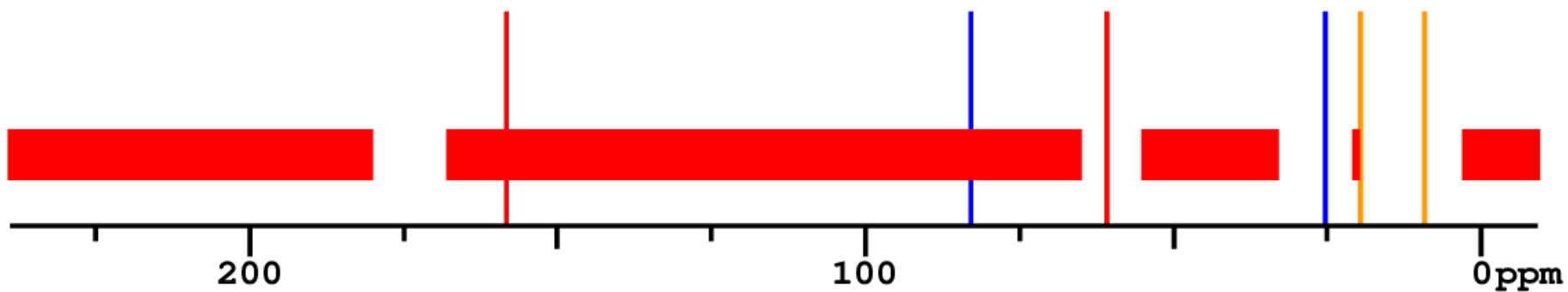
### Structure Proposal #10

Structure	Similarity Measure
	<p>Deviation = 9.45 ppm Similarity = 58 % (Different pattern)</p> <p><math>C_6H_{10}O</math></p> <p>MWT = 98.07</p> <p>Search Web for this structure: <a href="#">HUZIABIIFXMOH</a></p>
Predicted Chemical Shiftvalues	Matching Map



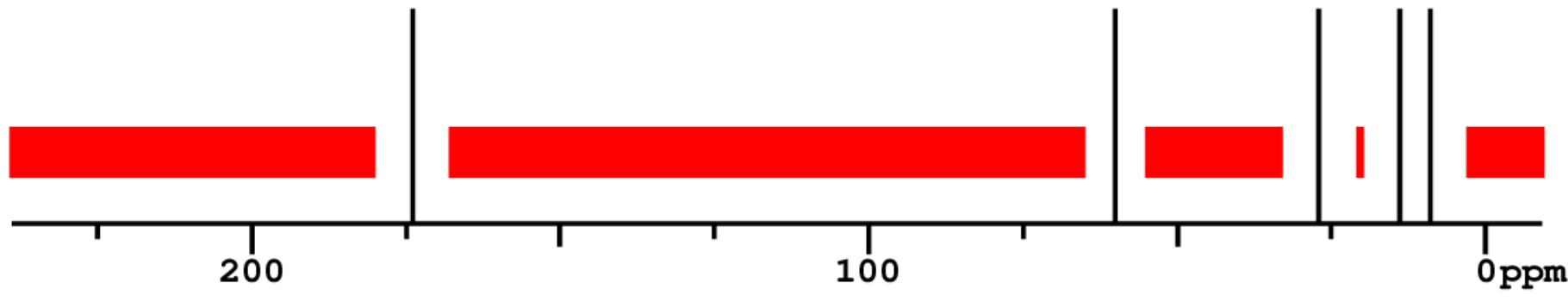
Predicted shift values

Signal multiplicity: **S****D****T****Q****O****E****P**?



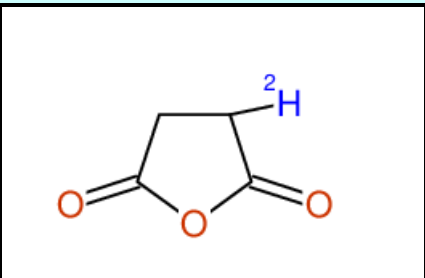
Experimental shift values

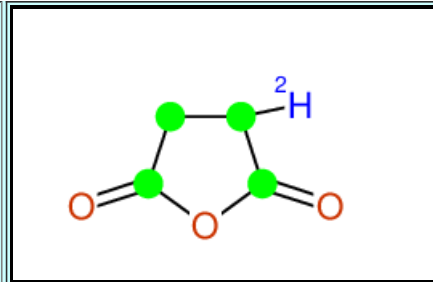
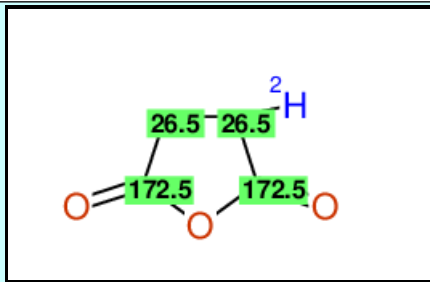
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[Back to Complete Result](#)

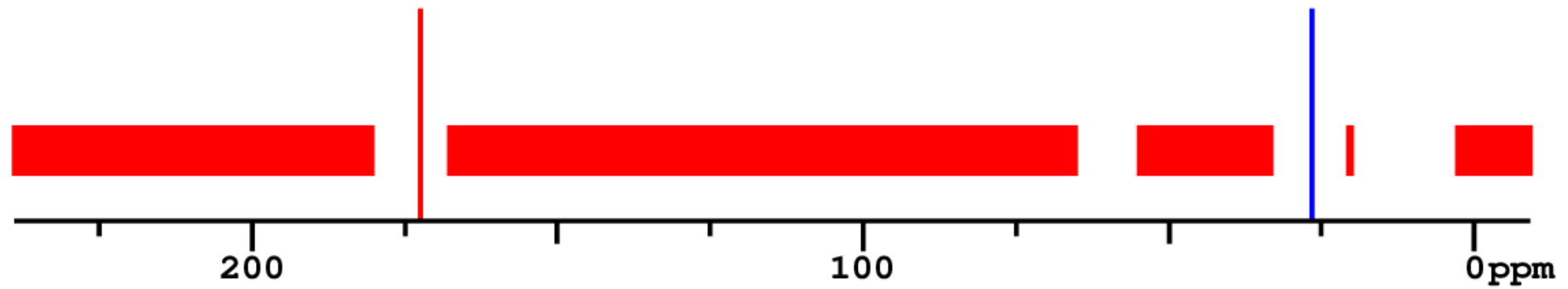
### Structure Proposal #11

Structure	Similarity Measure
	Deviation = 9.47 ppm Similarity = 100 %  C <sub>4</sub> H <sub>4</sub> O <sub>3</sub>  MWT = 101.04 Search Web for this structure: <a href="#">RINCXYOBBGOEEQ</a> <a href="#">Availability</a>
Predicted Chemical Shiftvalues	Matching Map



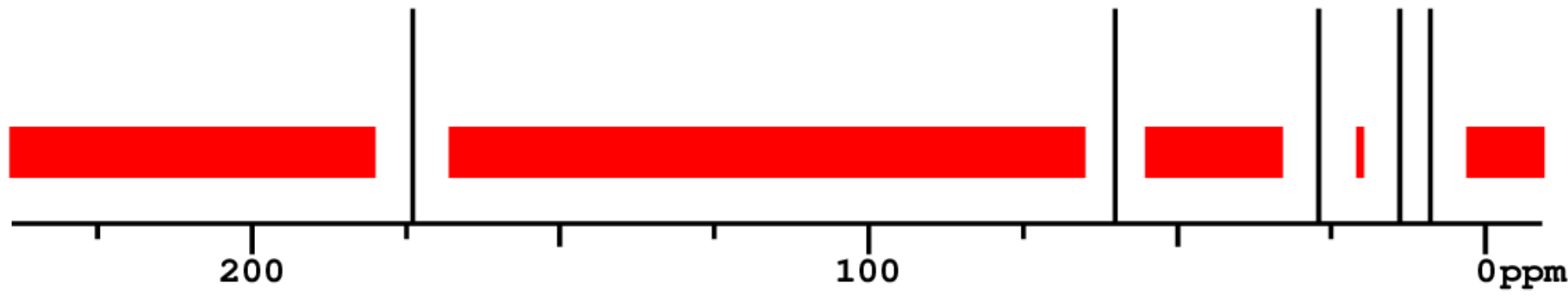
Predicted shift values

Signal multiplicity: **S****D****T****Q****O****E****P**?



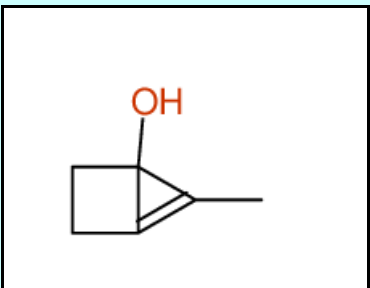
Experimental shift values

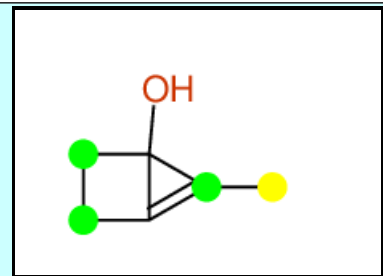
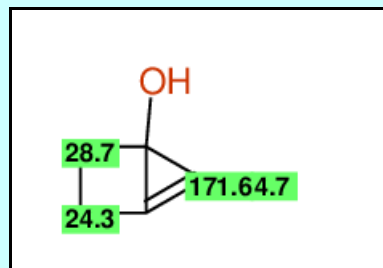
No line in reference: 



[Back to Complete Result](#)

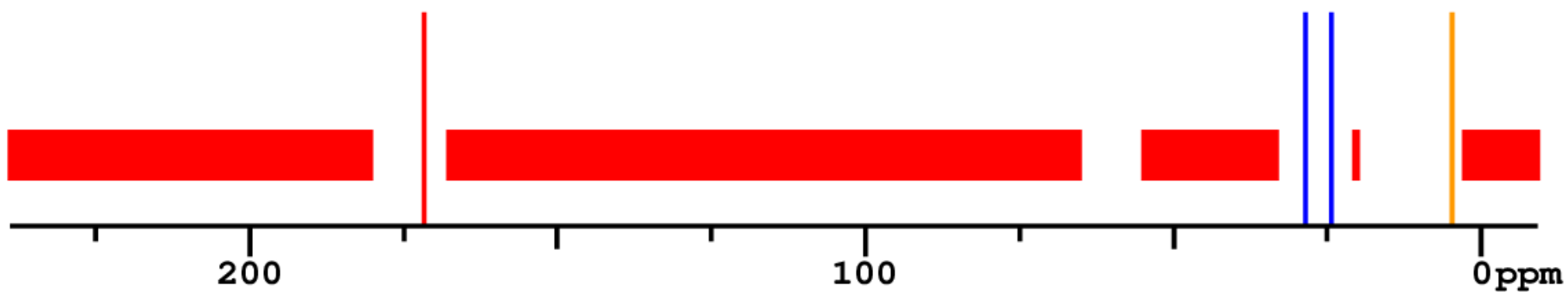
Structure Proposal #12

Structure	Similarity Measure
	<p>Deviation = 9.51 ppm Similarity = 88 %</p> <p><chem>C6H8O</chem></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">WPNREIWMCOZWLX</a></p>
Predicted Chemical Shiftvalues	Matching Map



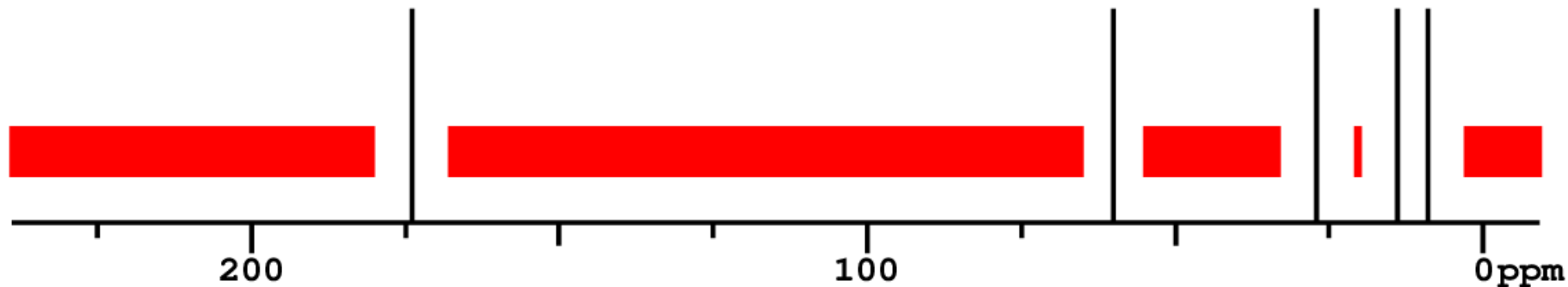
Predicted shift values

Signal multiplicity: S D T Q O E P ?



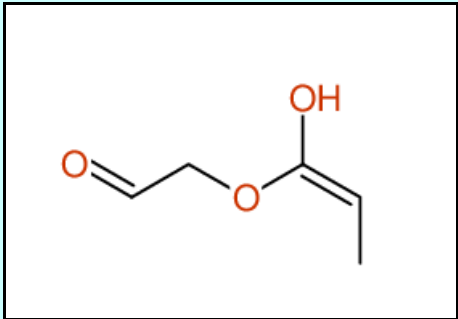
Experimental shift values

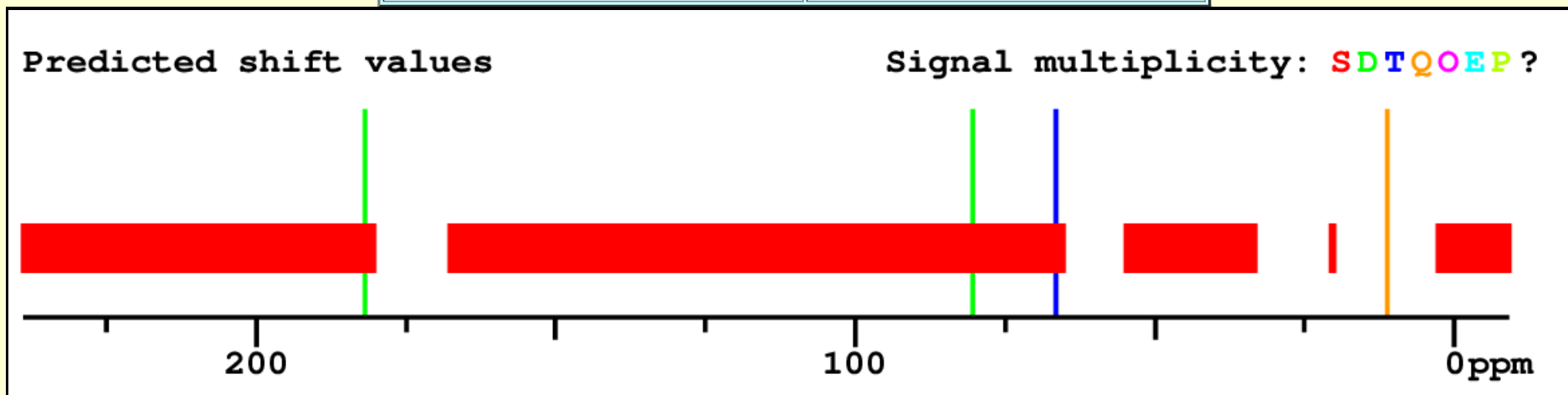
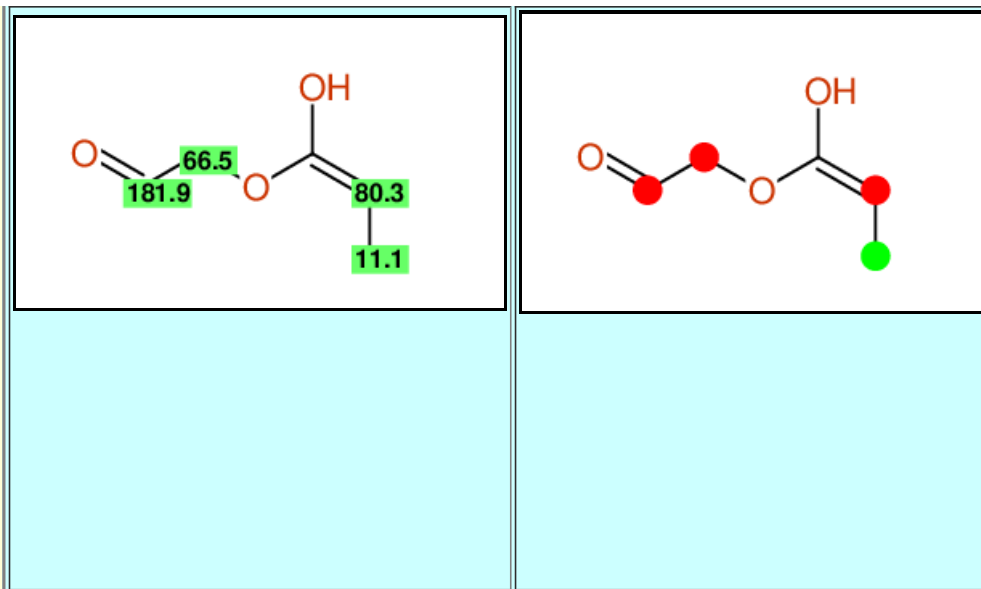
No line in reference: 



[Back to Complete Result](#)

### Structure Proposal #13

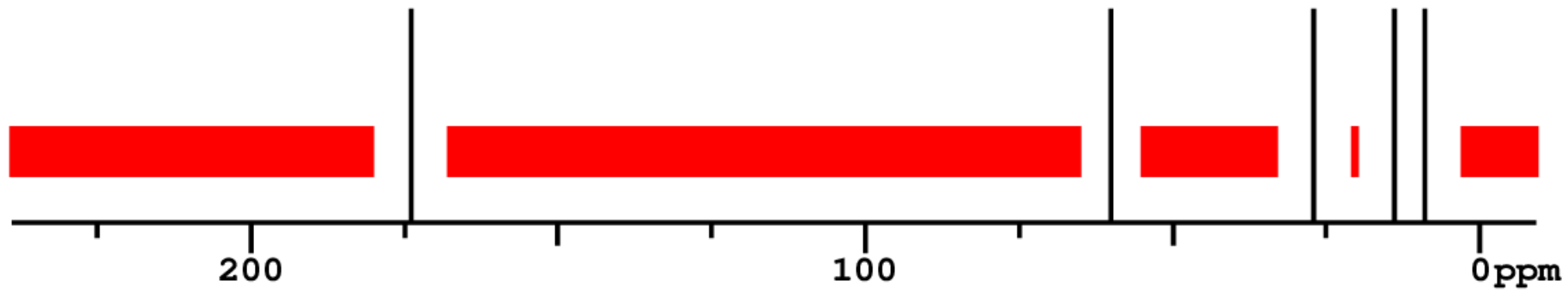
Structure	Similarity Measure
	<p>Deviation = 9.51 ppm Similarity = 25 % (Different pattern)</p> <p><math>C_5H_8O_3</math></p> <p>MWT = 116.06</p> <p>Search Web for this structure: <a href="#">LNDNUFLSISIDQD</a></p>
Predicted Chemical Shiftvalues	Matching Map





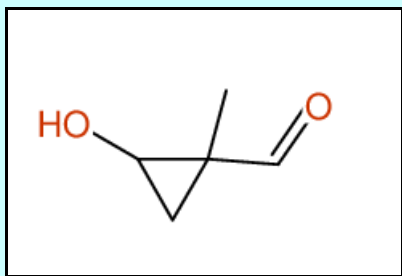
Experimental shift values

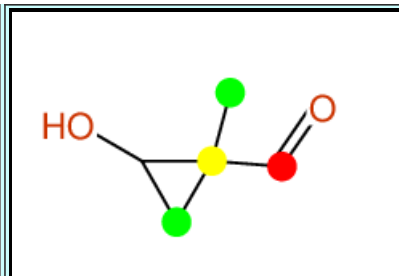
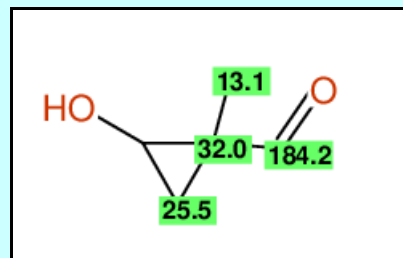
No line in reference: 



[Back to Complete Result](#)

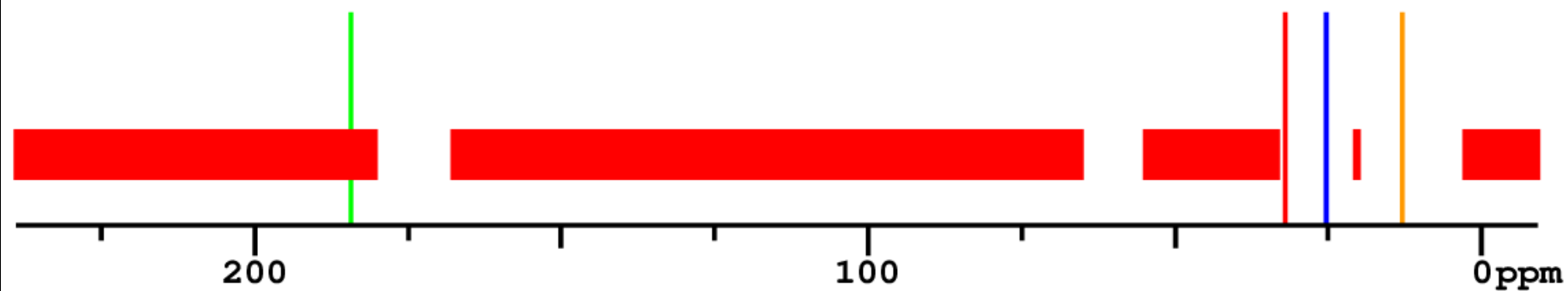
### Structure Proposal #14

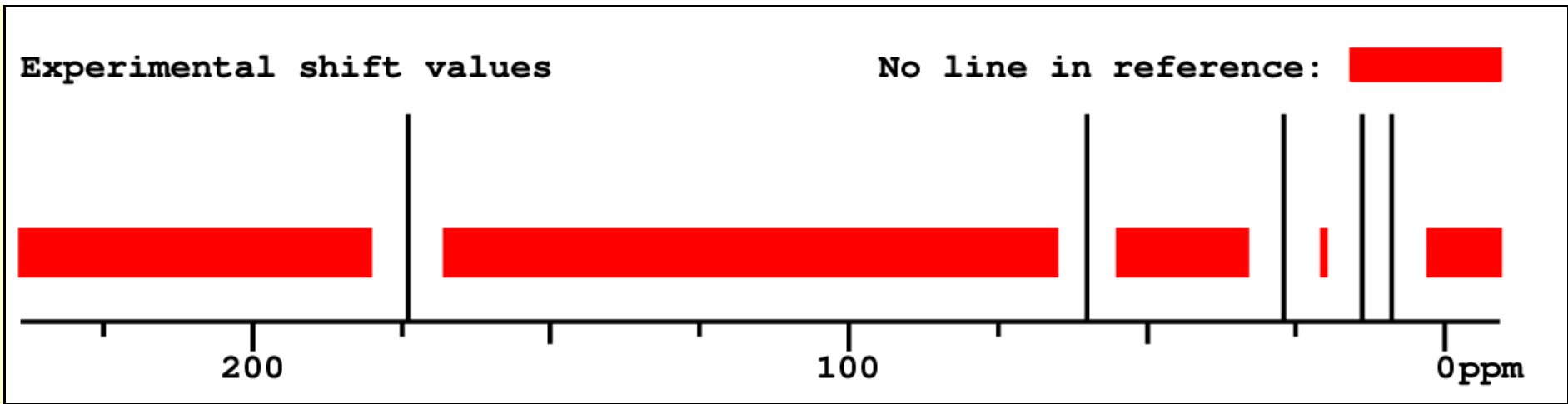
Structure	Similarity Measure
	<p>Deviation = 9.56 ppm Similarity = 63 % (Different pattern)</p> <p><math>C_5H_8O_2</math></p> <p>MWT = 100.06</p> <p>Search Web for this structure: <a href="#">ZOUPI LGYBSRVKU</a></p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

Signal multiplicity: S D T Q O E P ?





[Back to Complete Result](#)

Summary of the 2 most frequently occurring parent ring systems  
within the 2 best-fitting entries

Occurrence:

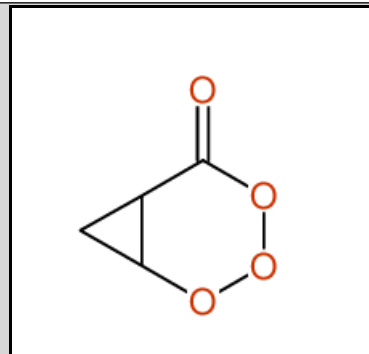
1 in 2

HO



Occurrence:

1 in 2



### Summary of Processing

Checking existence of data and counting them:	20,000,000 entries in 0.586 seconds
Applying restraints from elemental composition:	6.288 seconds, 510,515 entries remain
Applying restraints from number of signals:	0.446 seconds, 16,134 entries remain
Searching 299,998,280 chemical shift values line-per-line:	5.103 seconds
Best 4,229 entries selected for analysis:	0.567 seconds
Ranking of 4,229 entries by similarity:	49.518 seconds
Deviation of best match:	3.49 ppm
Creating table and linking 4,229 structures to 475,803 INCHIKEY-pages:	0.137 seconds
Detailed Analysis of 14 structures including graphical representation:	1.426 seconds

<b>Analysis of 2 structures for common parent ring systems:</b>	<b>0.007 seconds</b>
<b>Total CPU-usage:</b>	<b>64.253 seconds</b>
<b>Data transferred from disk:</b>	<b>1,234 MBytes out of 290,546 MBytes</b>
<b>Program version:</b>	<b>20200916_2-3D-zip/00</b>
<b>Machine:</b>	<b>I9-9900K / 16x3.60GHz</b>
<p><b>Page written by Wolfgang Robien using CSEARCH-Technology</b> <b>Page written on 2021:05:19 at 19:08</b> <b>Page finished on 2021:05:19 at 19:11</b></p> <p><b>Have a nice day !</b></p>	