

**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>

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:07

This page will be kept for 30 days here

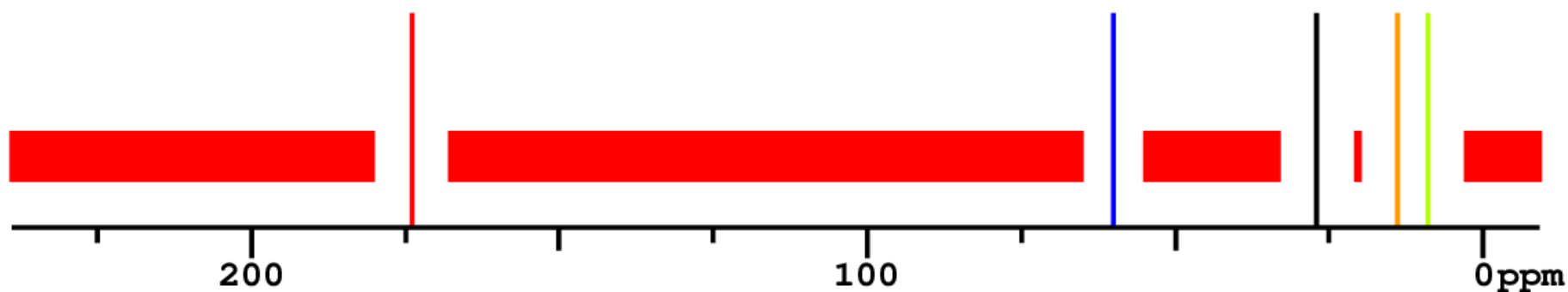
<b>Name of Project:</b>	<b>Test1</b>
<b>Comment:</b>	<b>Dereplication-engine</b>
<b>Name of Compound:</b>	<b>Propionic_acid,ethylester 400MHz</b>

### Summary of Supplied Data

Peaklist given - consists of 5 Lines				
Line number	Chemical Shift (ppm)	Multiplicity	Hydrogens	Deviation (ppm)
1	174.00	S	C	3.00
2	60.00	T	CH <sub>2</sub>	2.50
3	27.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00
4	14.00	Q	CH <sub>3</sub>	3.00
5	9.00	P	CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00

Experimental shift values

No line in reference: ████████



Additional Constraints given	
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	
Lower limit for molecular weight:	85.00
Upper limit for molecular weight:	120.00
N	Element must be absent
O	Element must be present

P	Element must be absent
S	Element must be absent
F	Element must be absent
Cl	Element must be absent
Br	Element must be absent
I	Element must be absent
other	Element must be absent

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

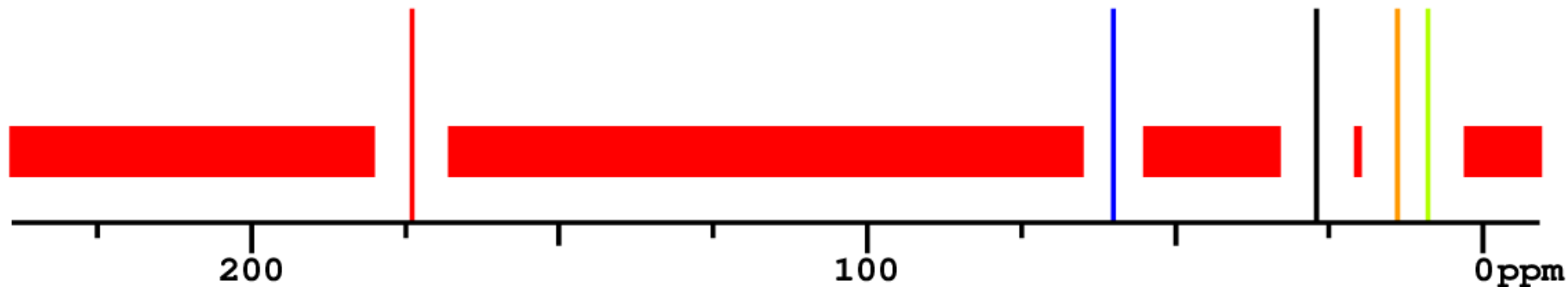
Available entries at each Screening-Step	
Total number of entries:	20,000,000

Applying requested elemental composition:	510,515 entries remain
Applying requested number of signals:	16,134 entries remain

Entries per line found out of 16,134 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	S	3.00	1,511	Impurity ?
2	60.00	T	2.50	1,463	Unspecific line
3	27.00	?	3.00	5,086	Unspecific line
4	14.00	Q	3.00	2,296	Impurity ?
5	9.00	P	3.00	2,617	Unspecific line

Experimental shift values

No line in reference: ████████

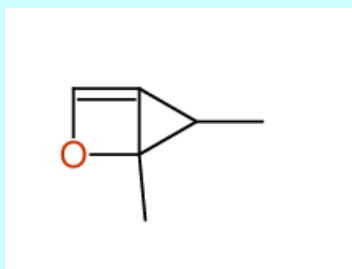


Number of coincident lines versus number of entries		
Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	1	Selected for detailed analysis
4	44	Selected for detailed analysis
3	401	Selected for detailed analysis
2	2,440	Selected for detailed analysis
1	6,709	

Best 20 Proposals shown for Compound: Propionic\_acid,ethylester::400MHz

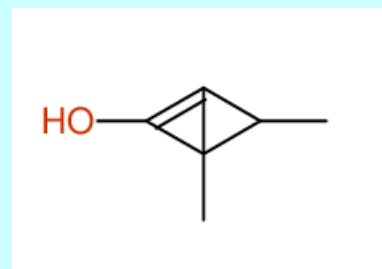
3.82 -  
3.82ppm

1x found [QHOFHRHGMVSHCQ](#)



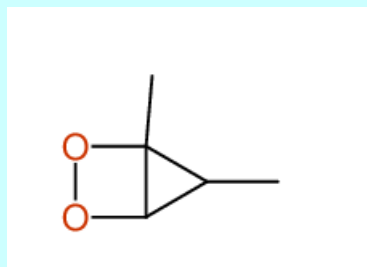
3.85 -  
3.85ppm

1x found [PHPVAGXZXAHNIJ](#)



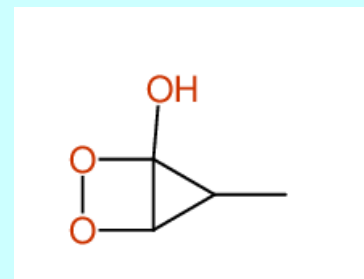
3.85 -  
3.85ppm

1x found [ZLXIQGKKYBVHAW](#)



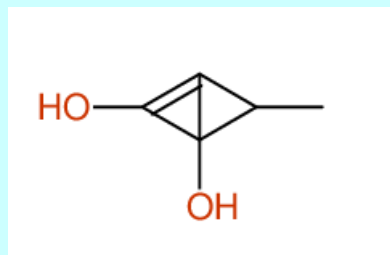
3.94 -  
3.94ppm

1x found [JGBLVVQAZJCZED](#)



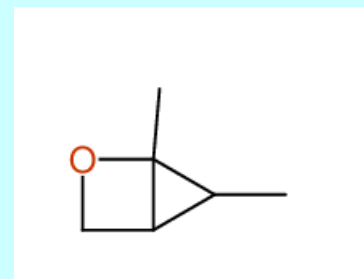
4.24 -  
4.24ppm

1x found [YLBSGXAZACMXQK](#)



4.28 -  
4.28ppm

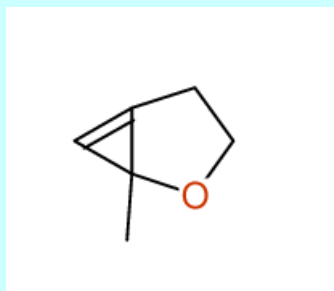
1x found [RRUPDGSLWBNUSW](#)



4.46 -  
4.46ppm

1x found

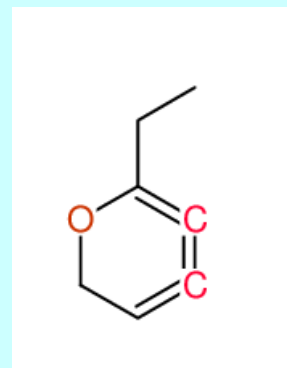
[MLKQXIPGHOLEQI](#)



4.60 -  
4.60ppm

1x found

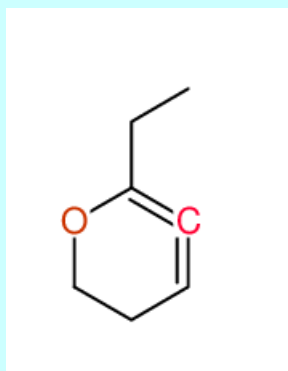
[PNZSQYMQKDYYDJ](#)



4.70 -  
4.70ppm

1x found

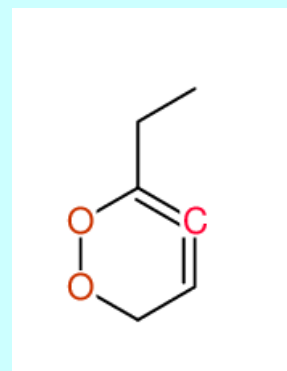
[DRDGAMGKENXWCN](#)



4.72 -  
4.72ppm

1x found

[HQZWXOPRWOPVAU](#)

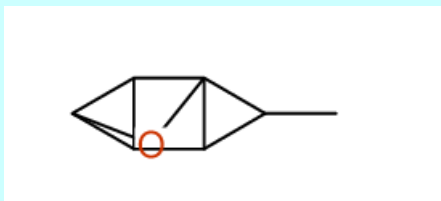




4.78 -  
4.78ppm

1x found

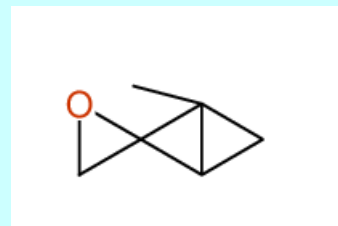
[RPKFSYMKPKZHO](#)



4.90 -  
4.90ppm

1x found

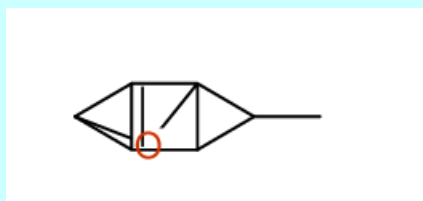
[LOABURPYMMQUIT](#)



5.10 -  
5.10ppm

1x found

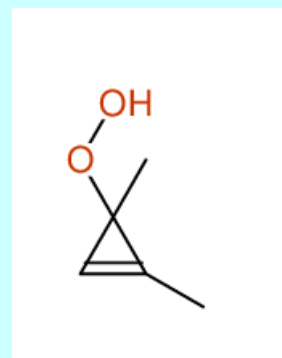
[HDESMDVUQOYCMC](#)



5.12 -  
5.12ppm

1x found

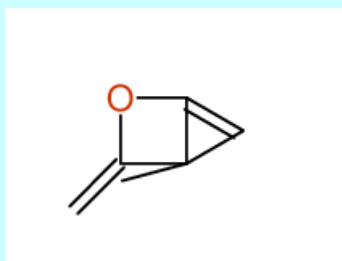
[QJQMTQIRFXBQEU](#)



5.87 -  
5.87ppm

1x found

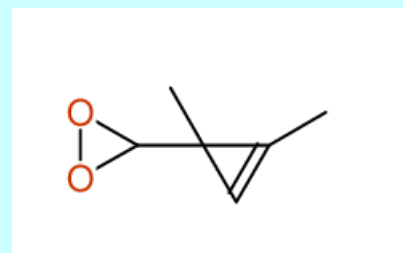
[YDMXGLHNPWXWND](#)



5.92 -  
5.92ppm

1x found

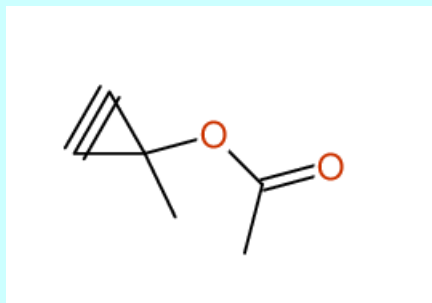
[AFXAYZSYHSLEGG](#)



5.94 -  
5.94ppm

1x found

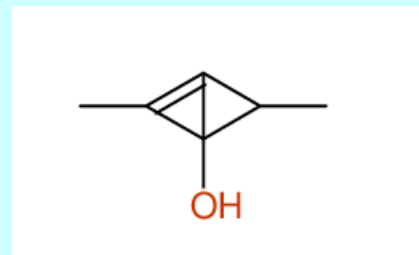
[UBJMOXHHNZUDRL](#)



6.26 -  
6.26ppm

1x found

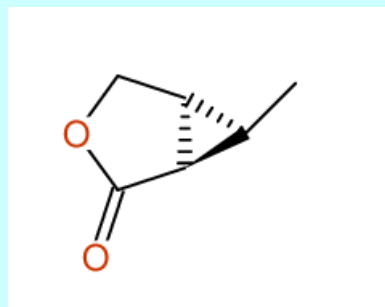
[HBGRMNFFAOTRDL](#)



6.45 -  
6.45ppm

1x found

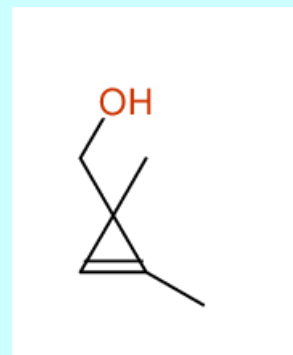
[ODZSNSOKRZBPDY](#)



6.70 -  
6.70ppm

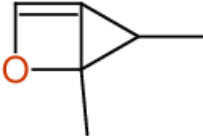
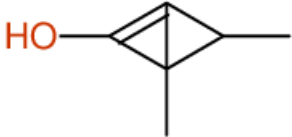
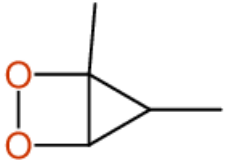
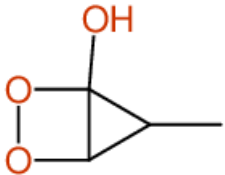
1x found

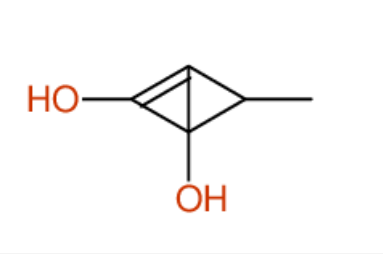
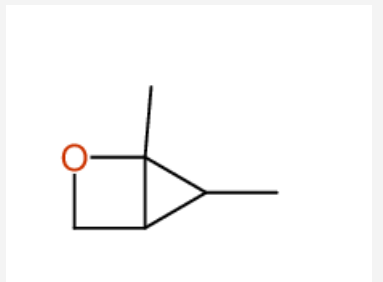

[XDZLYFBRUGYBSU](#)

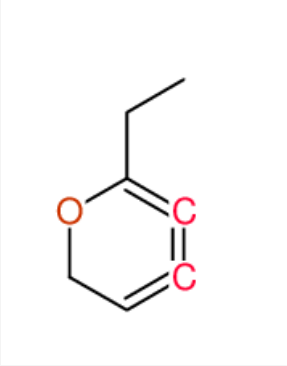
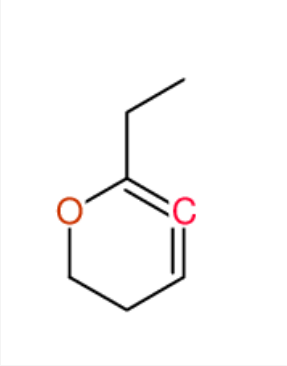


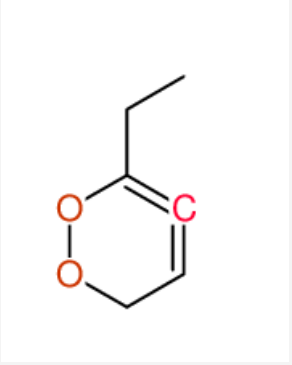
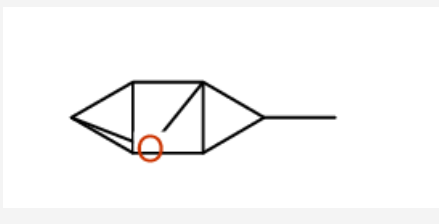
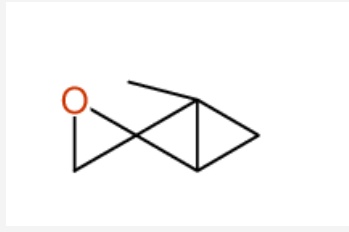
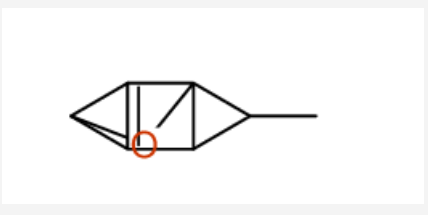
2,886 [Structure proposals](#) found for your C-NMR Spectrum

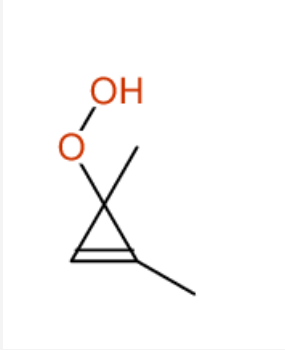
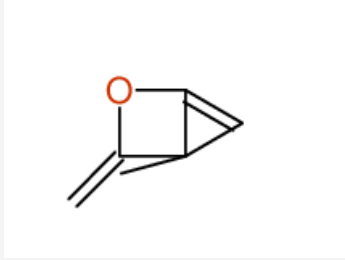
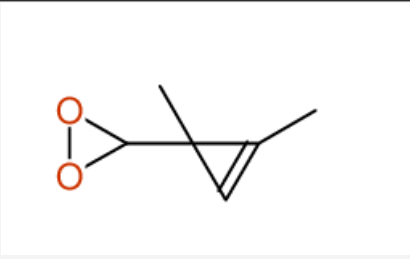
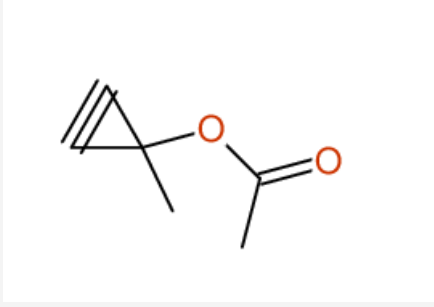
266 Entries will be shown because of your selection of additional constraints

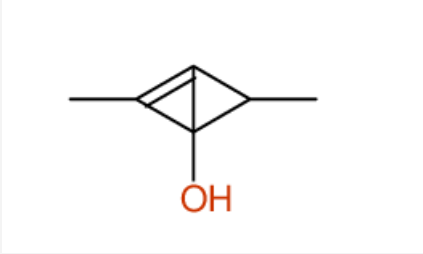
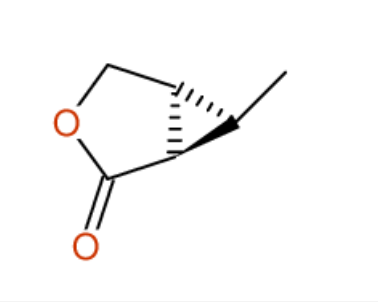
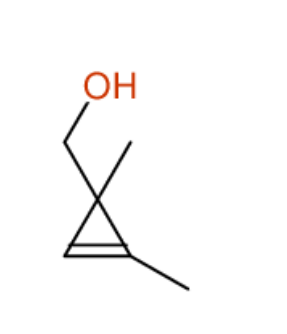
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1  3.82  <a href="#">Details</a>		$C_6H_8O$ MWT = 96.066	Proposal #1 Structure-ID: 16,814,871 <a href="#">QHOFHRHGVMVSHCQ-UHFFFAOYAY</a>	
Proposal #2  3.85  <a href="#">Details</a>		$C_6H_8O$ MWT = 96.066	Proposal #2 Structure-ID: 16,816,700 <a href="#">PHPVAGXZXAHNIJ-UHFFFAOYAN</a>	
Proposal #3  3.85  <a href="#">Details</a>		$C_5H_8O_2$ MWT = 100.055	Proposal #3 Structure-ID: 16,815,127 <a href="#">ZLXIQQKKYBVHAW-UHFFFAOYAZ</a>	
Proposal #4  3.94  <a href="#">Details</a>		$C_4H_6O_3$ MWT = 102.044	Proposal #4 Structure-ID: 16,815,129 <a href="#">JGBLVVQAZJCZED-UHFFFAOYAA</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #5</p> <p>4.24</p> <p><a href="#">Details</a></p>		<p>C<sub>5</sub>H<sub>6</sub>O<sub>2</sub></p> <p>MWT = 98.055</p>	<p>Proposal #5</p> <p>Structure-ID: 16,816,702</p> <p><a href="#">YLBGXAZACMXQK-UHFFFAOYAC</a></p>	
<p>Proposal #6</p> <p>4.28</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p>C<sub>6</sub>H<sub>10</sub>O</p> <p>MWT = 98.066</p>	<p>Proposal #6</p> <p>Structure-ID: 16,815,109</p> <p><a href="#">RRUPDGSLWBNUSW-UHFFFAOYAC</a></p>	
<p>Proposal #7</p> <p>4.46</p> <p><a href="#">Details</a></p>		<p>C<sub>6</sub>H<sub>8</sub>O</p> <p>MWT = 96.066</p>	<p>Proposal #7</p> <p>Structure-ID: 16,816,150</p> <p><a href="#">MLKQXIPGHOLEQI-UHFFFAOYAA</a></p>	

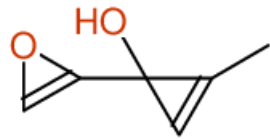
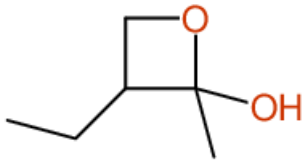
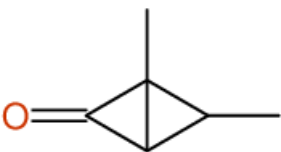
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #8</p> <p>4.60</p> <p><a href="#">Details</a></p>		<p><math>C_7H_8O</math></p> <p>MWT = 108.077</p>	<p>Proposal #8</p> <p>Structure-ID: 17,032,651</p> <p><a href="#">PNZSQYMQDYDJ-UHFFFAOYAP</a></p>	
<p>Proposal #9</p> <p>4.70</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 #9</p> <p>Structure-ID: 17,033,224</p> <p><a href="#">DRDGAMGKENXWCN-UHFFFAOYAL</a></p>	

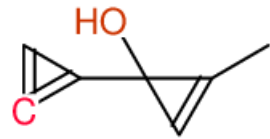
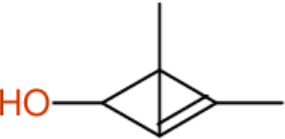
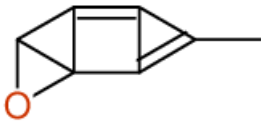

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #10</p> <p>4.72</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_8O_2</math></p> <p>MWT = 112.066</p>	<p>Proposal #10</p> <p>Structure-ID: 17,033,230</p> <p><a href="#">HQZWXOPRWOPVAU-UHFFFAOYAG</a></p>	
<p>Proposal #11</p> <p>4.78</p> <p><a href="#">Details</a></p>		<p><math>C_7H_8O</math></p> <p>MWT = 108.077</p>	<p>Proposal #11</p> <p>Structure-ID: 844,269</p> <p><a href="#">RPKFKSYMCPKZHO-UHFFFAOYAF</a></p>	
<p>Proposal #12</p> <p>4.90</p> <p><a href="#">Details</a></p>		<p><math>C_6H_8O</math></p> <p>MWT = 96.066</p>	<p>Proposal #12</p> <p>Structure-ID: 674,786</p> <p><a href="#">LOABURPYMMQUIT-UHFFFAOYAS</a></p>	
<p>Proposal #13</p> <p>5.10</p> <p><a href="#">Details</a></p>		<p><math>C_7H_8O</math></p> <p>MWT = 106.077</p>	<p>Proposal #13</p> <p>Structure-ID: 844,120</p> <p><a href="#">HDESMDVUQOYCMC-UHFFFAOYAH</a></p>	

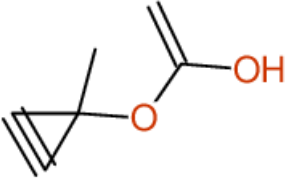
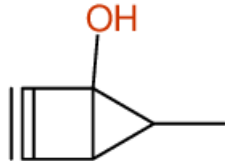
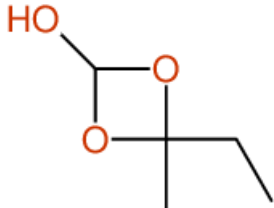
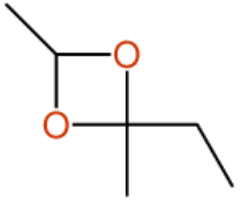
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #14</p> <p>5.12</p> <p><a href="#">Details</a></p>		<p><math>C_5H_8O_2</math></p> <p>MWT = 100.055</p>	<p>Proposal #14</p> <p>Structure-ID: 17,071,647</p> <p><a href="#">QJQMTQIRFXBQEU-UHFFFAOYAP</a></p>	
<p>Proposal #15</p> <p>5.87</p> <p><a href="#">Details</a></p>		<p><math>C_6H_6O</math></p> <p>MWT = 94.066</p>	<p>Proposal #15</p> <p>Structure-ID: 16,816,889</p> <p><a href="#">YDMXGLHNPWXWND-UHFFFAOYAS</a></p>	
<p>Proposal #16</p> <p>5.92</p> <p><a href="#">Details</a></p>		<p><math>C_6H_8O_2</math></p> <p>MWT = 112.066</p>	<p>Proposal #16</p> <p>Structure-ID: 16,988,908</p> <p><a href="#">AFXAYZSYHSLEGG-UHFFFAOYAR</a></p>	
<p>Proposal #17</p> <p>5.94</p> <p><a href="#">Details</a></p>		<p><math>C_6H_6O_2</math></p> <p>MWT = 110.066</p>	<p>Proposal #17</p> <p>Structure-ID: 864,071</p> <p><a href="#">UBJMOXHHNZUDRL-UHFFFAOYAV</a></p>	

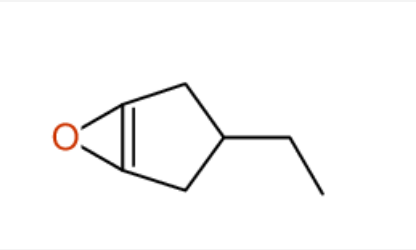
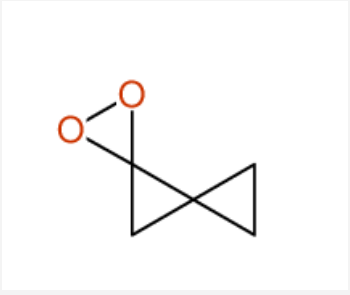
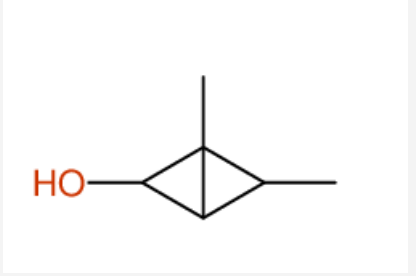
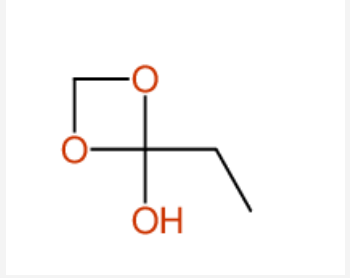
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<p>Proposal #19</p> <p>6.45</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_8O_2</math></p> <p>MWT = 112.066</p>	<p>Proposal #19</p> <p>Structure-ID: 18,263,141</p> <p><a href="#">ODZSNSOKRZBPDY-LJJLCWGRBL</a></p>	
<p>Proposal #20</p> <p>6.70</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 #20</p> <p>Structure-ID: 17,071,643</p> <p><a href="#">XDZLYFBRUGYBSU-UHFFFAOYAJ</a></p>	

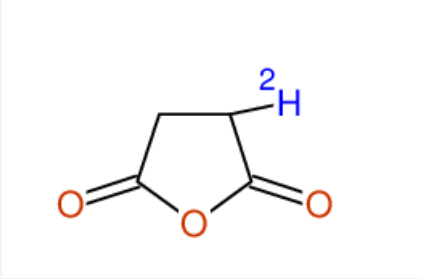

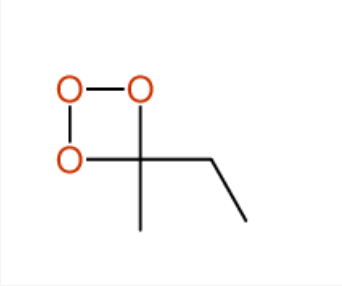
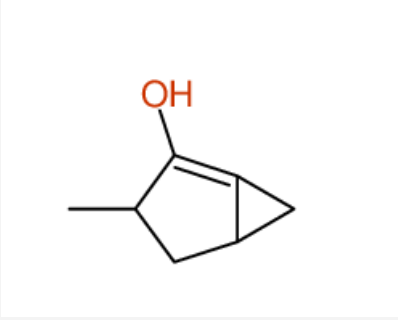


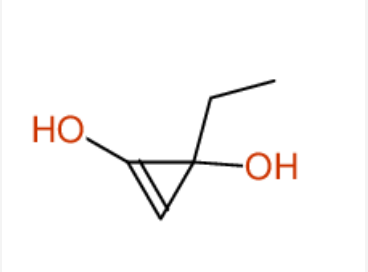
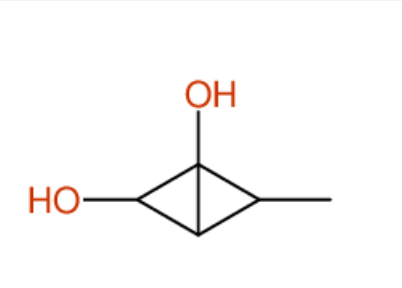
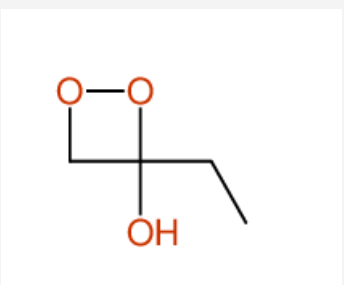
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Proposal #22  6.89  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #22 Structure-ID: 702,071 <a href="#">DHCRDJAGJXWNRZ-UHFFFAOYAX</a>	
Proposal #23  7.00  <a href="#">Details</a>  Different pattern		$C_6H_8O$ MWT = 96.066	Proposal #23 Structure-ID: 16,816,741 <a href="#">SXZKEFLVORMPAX-UHFFFAOYAR</a>	

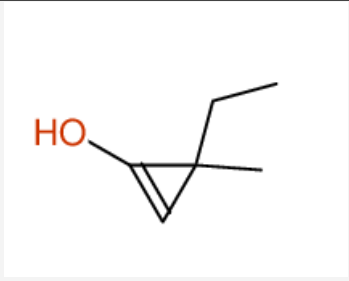
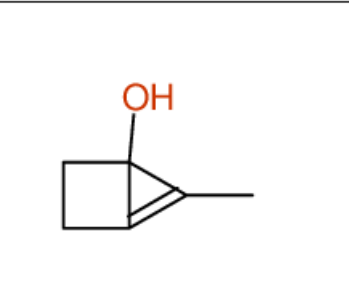
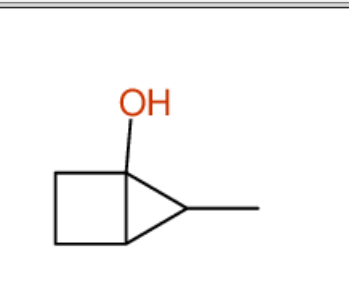
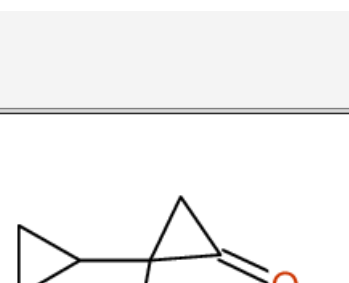
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Proposal #25  7.25  <a href="#">Details</a>  Different pattern		$C_6H_8O$ MWT = 96.066	Proposal #25 Structure-ID: 16,816,686 <a href="#">RJYJUVCQXAQWHG-UHFFFAOYAV</a>	
Proposal #26  7.49  <a href="#">Details</a>  Different pattern		$C_7H_4O$ MWT = 104.077	Proposal #26 Structure-ID: 845,578 <a href="#">XYXRSMOQFNPFQ-UHFFFAOYAW</a>	
Proposal #27  7.82  <a href="#">Details</a>		$C_7H_4O$ MWT = 104.077	Proposal #27 Structure-ID: 844,004 <a href="#">YXVQMKXJOHSUEX-UHFFFAOYAX</a>	

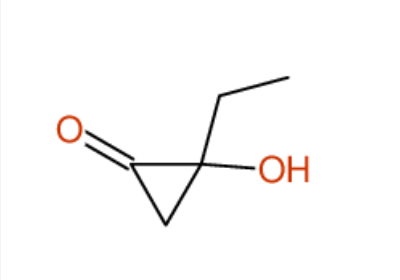
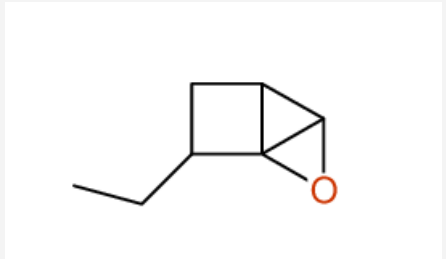
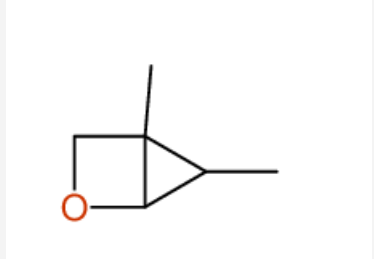
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Proposal #28  8.16  <a href="#">Details</a>		$C_6H_6O_2$ MWT = 110.066	Proposal #28 Structure-ID: 864,087 <a href="#">QYPIJZABARONQ-UHFFFAOYAP</a>	
Proposal #29  8.28  <a href="#">Details</a>  Different pattern		$C_6H_{12}O$ MWT = 94.066	Proposal #29 Structure-ID: 16,814,919 <a href="#">GJAGHYKQEPSPNN-UHFFFAOYAR</a>	
Proposal #30  8.34  <a href="#">Details</a>  Different pattern		$C_5H_{10}O_3$ MWT = 118.055	Proposal #30 Structure-ID: 863,479 <a href="#">CMMVOYHDZZWOKB-UHFFFAOYAX</a>	
Proposal #31  8.49  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #31 Structure-ID: 863,477 <a href="#">HRHKYDWQVMBLPA-UHFFFAOYAR</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #32  8.74  <a href="#">Details</a>  Different pattern		$C_7H_{10}O$ MWT = 110.077	Proposal #32 Structure-ID: 17,258,756 <a href="#">SIFWESXVNIJEJB-UHFFFAOYAY</a>	
Proposal #33  8.75  <a href="#">Details</a>		$C_5H_6O_2$ MWT = 98.055	Proposal #33 Structure-ID: 674,960 <a href="#">WGAVRTDGCNTZGM-UHFFFAOYAU</a>	
Proposal #34  8.75  <a href="#">Details</a>		$C_6H_{10}O$ MWT = 98.066	Proposal #34 Structure-ID: 16,816,815 <a href="#">NEQPKAVUXMOCHO-UHFFFAOYAA</a>	
Proposal #35  8.90  <a href="#">Details</a>		$C_4H_8O_3$ MWT = 104.044	Proposal #35 Structure-ID: 17,069,844 <a href="#">CIDICLGXRQBWBQ-UHFFFAOYAL</a>	

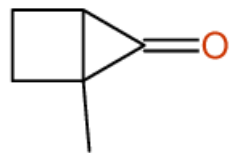
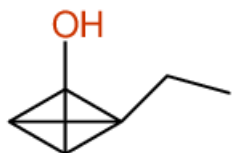
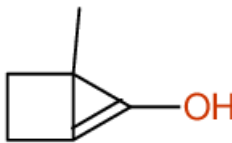
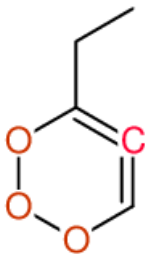
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<b>Proposal #36</b>  9.10 <a href="#">Details</a>		$C_4H_4O_3$ MWT = 101.044	Proposal #36 Structure-ID: 7,029,234 <a href="#">RINCXYDBBGOEQ-MICDWDOJEO</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH 
<b>Proposal #37</b>  9.11 <a href="#">Details</a>		$C_4H_8O_3$ MWT = 104.044	Proposal #37 Structure-ID: 17,069,817 <a href="#">CZUKTAOOHAZAPX-UHFFFAOYAJ</a>	
<b>Proposal #38</b>  9.12 <a href="#">Details</a> Different pattern		$C_7H_{10}O$ MWT = 110.077	Proposal #38 Structure-ID: 654,774 <a href="#">WQZCEYRBPLRVQT-UHFFFAOYAN</a>	


Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #39</p> <p>9.17</p> <p><a href="#">Details</a></p>		<p><math>C_5H_8O_2</math></p> <p>MWT = 100.055</p>	<p>Proposal #39</p> <p>Structure-ID: 17,071,691</p> <p><a href="#">LYEDKJATIQMCTQ-UHFFFAOYAY</a></p>	
<p>Proposal #40</p> <p>9.31</p> <p><a href="#">Details</a></p>		<p><math>C_5H_8O_2</math></p> <p>MWT = 100.055</p>	<p>Proposal #40</p> <p>Structure-ID: 16,816,817</p> <p><a href="#">XLPULUZDFMTOLL-UHFFFAOYAZ</a></p>	
<p>Proposal #41</p> <p>9.40</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_4H_8O_3</math></p> <p>MWT = 104.044</p>	<p>Proposal #41</p> <p>Structure-ID: 17,069,837</p> <p><a href="#">LPMMUOPZFPDUGT-UHFFFAOYAF</a></p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #42  9.40  <a href="#">Details</a>		$C_6H_{10}O$ MWT = 98.066	Proposal #42 Structure-ID: 17,071,679 <a href="#">NTSMDFJAQBLTSB-UHFFFAOYAQ</a>	
Proposal #43  9.51  <a href="#">Details</a>		$C_6H_8O$ MWT = 96.066	Proposal #43 Structure-ID: 16,814,789 <a href="#">WPNREIWMCOZWLX-UHFFFAOYAR</a>	
Proposal #44  9.58  <a href="#">Details</a>		$C_6H_{10}O$ MWT = 98.066	Proposal #44 Structure-ID: 16,815,105 <a href="#">JXAXUPPGOOMCOO-UHFFFAOYAW</a>	
Proposal #45  9.63  <a href="#">Details</a>		$C_7H_{10}O$ MWT = 110.077	Proposal #45 Structure-ID: 16,988,452 <a href="#">IXMZEVVZABSMMG-UHFFFAOYAT</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #46</p> <p>9.65</p> <p><a href="#">Details</a></p>		<p><math>C_5H_8O_2</math></p> <p>MWT = 100.055</p>	<p>Proposal #46</p> <p>Structure-ID: 17,071,800</p> <p><a href="#">GTNDLTKJPEYUIS-UHFFFAOYAR</a></p>	
<p>Proposal #47</p> <p>9.66</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 #47</p> <p>Structure-ID: 692,545</p> <p><a href="#">SUBRYTRHWOBQI-UHFFFAOYAH</a></p>	
<p>Proposal #48</p> <p>9.71</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 #48</p> <p>Structure-ID: 16,815,121</p> <p><a href="#">IPPBHXUICADJGT-UHFFFAOYAX</a></p>	

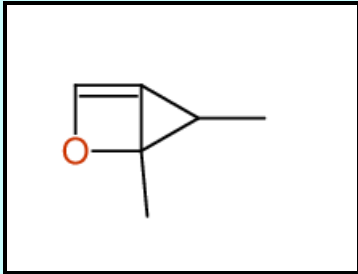


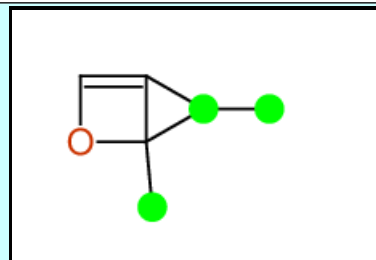
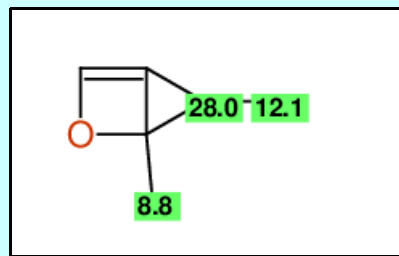
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<b>Proposal #49</b>  9.76 <a href="#">Details</a>		$C_6H_8O$ MWT = 96.066	<b>Proposal #49</b> Structure-ID: 16,814,633 <a href="#">ORTSZOHNPUCPJW-UHFFFAOYAX</a>	
<b>Proposal #50</b>  9.85 <a href="#">Details</a>		$C_6H_8O$ MWT = 96.066	<b>Proposal #50</b> Structure-ID: 674,652 <a href="#">LFNUXUXAOVSIAA-UHFFFAOYAZ</a>	
<b>Proposal #51</b>  9.91 <a href="#">Details</a> Different pattern		$C_6H_8O$ MWT = 96.066	<b>Proposal #51</b> Structure-ID: 16,814,771 <a href="#">QNDKYNSAESMQHX-UHFFFAOYAO</a>	
<b>Proposal #52</b>  10.01		$C_5H_6O_3$ MWT = 114.055	<b>Proposal #52</b> Structure-ID: 17,033,248 <a href="#">BJPIUGZDTJYXGB-UHFFFAOYAK</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #53  10.04		$C_5H_6O_3$ MWT = 114.055	Proposal #53 Structure-ID: 16,988,457 <a href="#">PZGAHQRWJBZOSA-UHFFFAOYAG</a>	

## Detailed Analysis

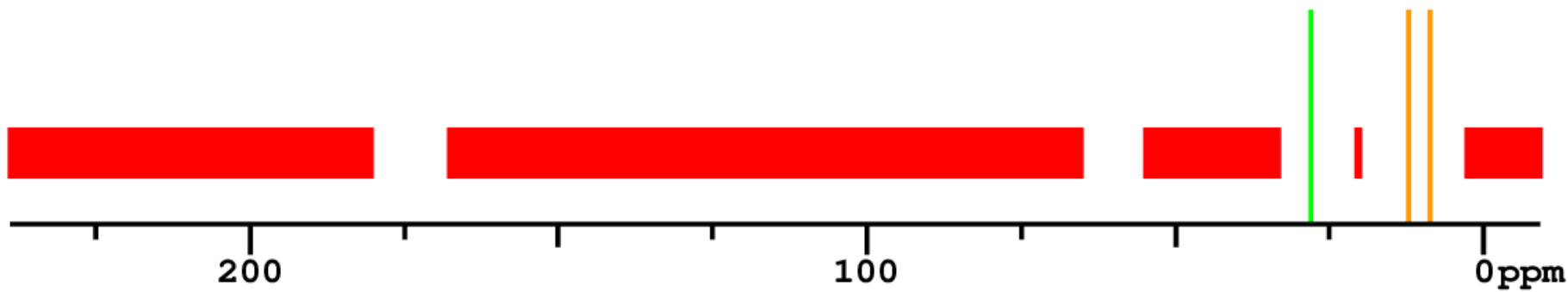
### Structure Proposal #1

Structure	Similarity Measure
	Deviation = 3.82 ppm Similarity = 100 %  $C_6H_8O$ MWT = 96.07 Search Web for this structure: <a href="#">QHOFHRHGMVSHCO</a>
Predicted Chemical Shiftvalues	Matching Map



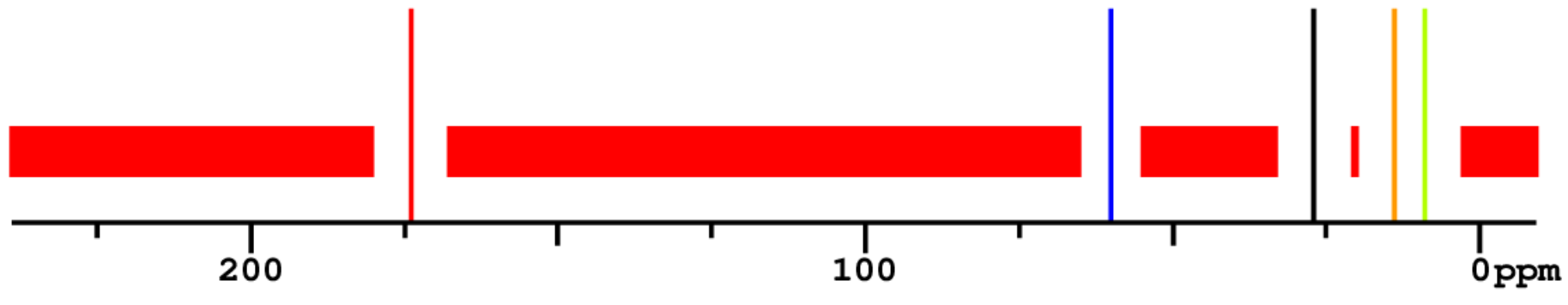
Predicted shift values

Signal multiplicity: S D T Q O E P ?



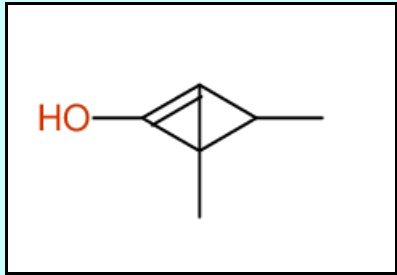
Experimental shift values

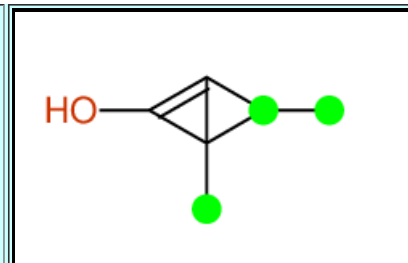
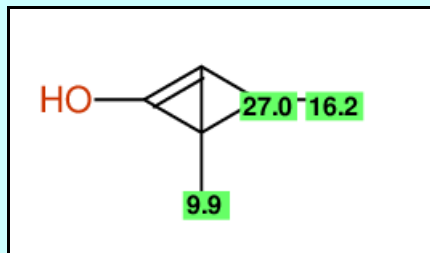
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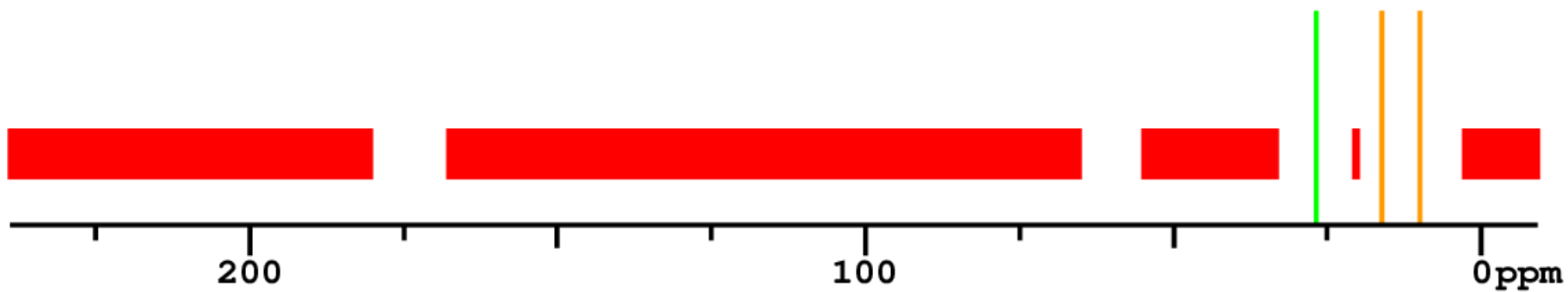
### Structure Proposal #2

Structure	Similarity Measure
	Deviation = 3.85 ppm Similarity = 100 %  $C_6H_8O$  MWT = 96.07 Search Web for this structure: <a href="#">PHPVAGXZXAHNIJ</a>
Predicted Chemical Shiftvalues	Matching Map



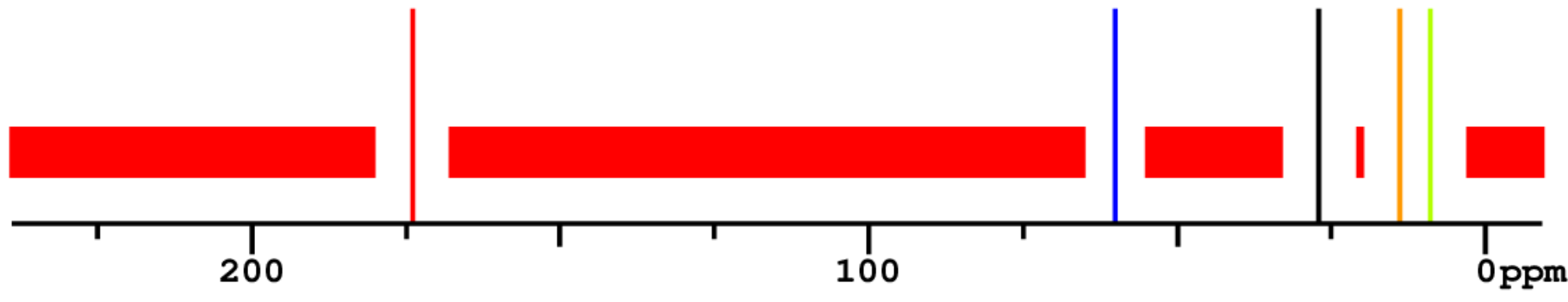
Predicted shift values

Signal multiplicity: S D T Q O E P ?



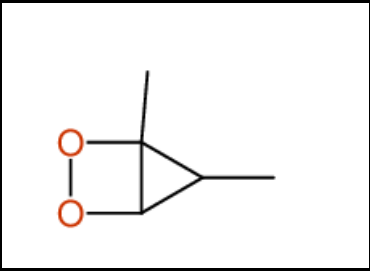
Experimental shift values

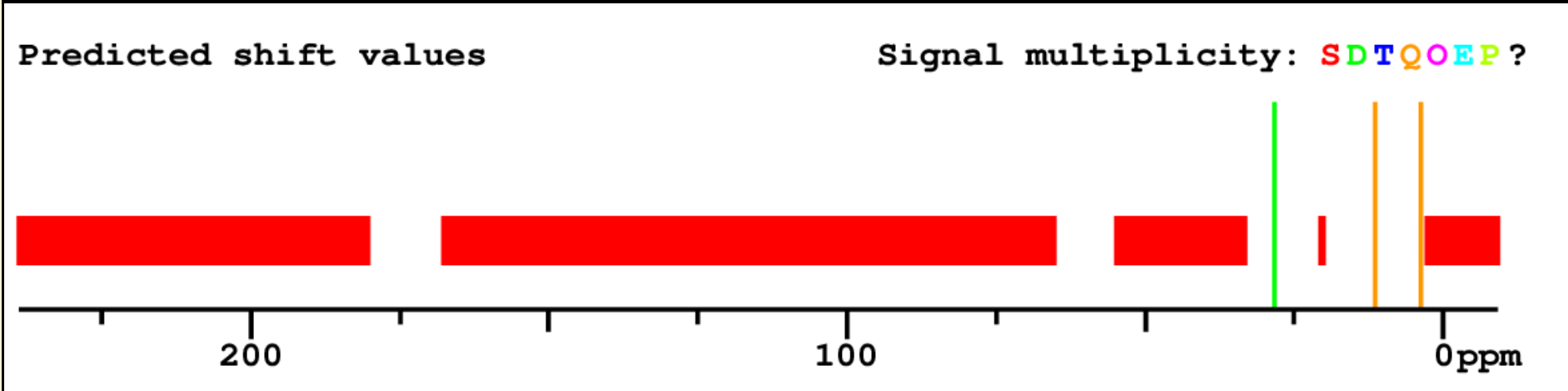
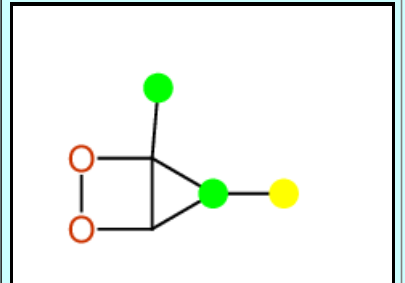
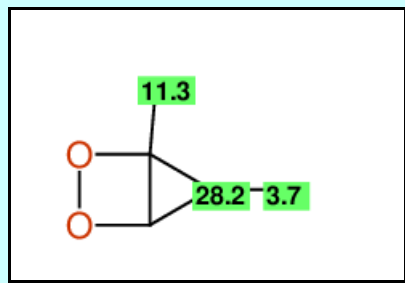
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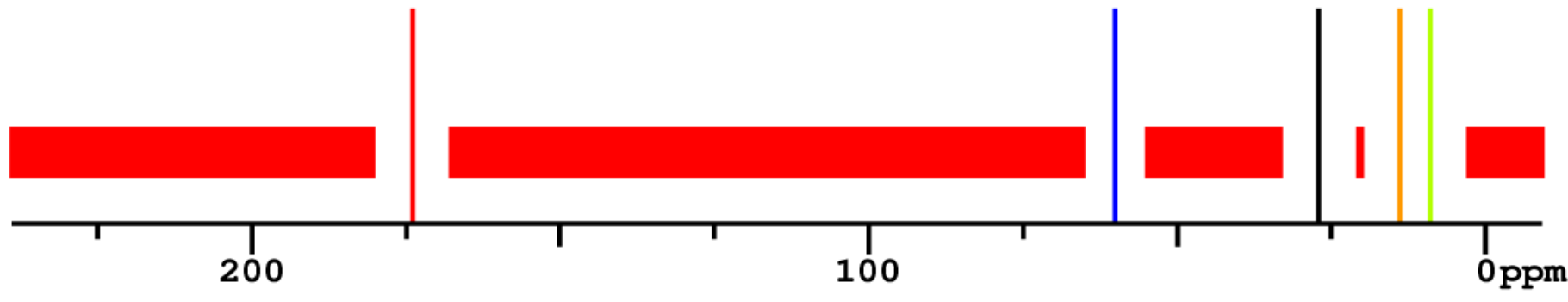
### Structure Proposal #3

Structure	Similarity Measure
	<p>Deviation = 3.85 ppm Similarity = 83 %</p> <p><math>C_5H_8O_2</math></p> <p>MWT = 100.06</p> <p>Search Web for this structure: <a href="#">ZLXIQQKKYBVHAW</a></p>
<p>Predicted Chemical Shiftvalues</p>	<p>Matching Map</p>



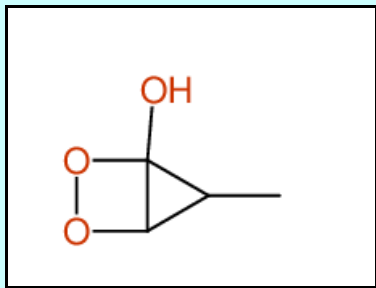
Experimental shift values

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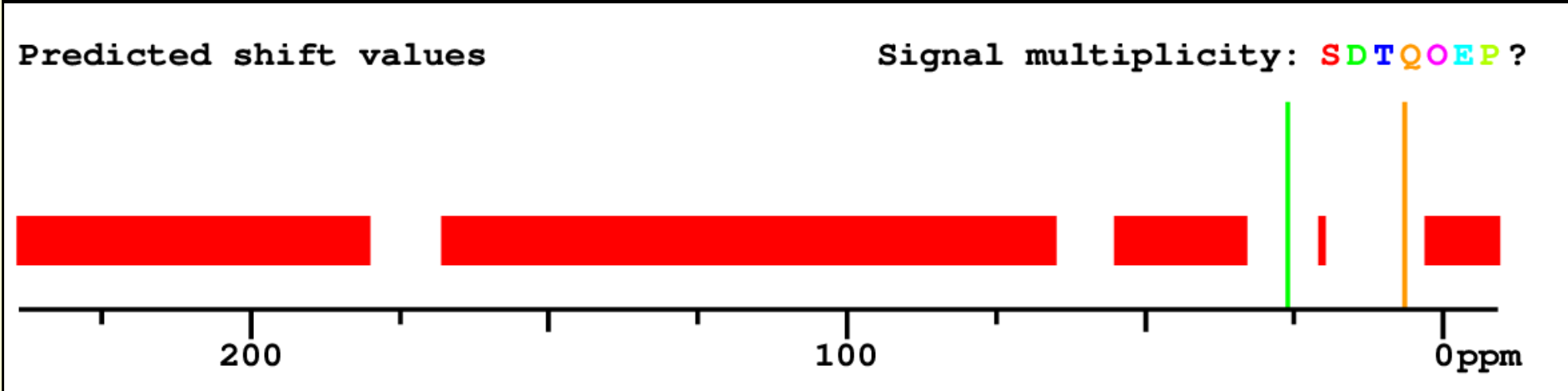
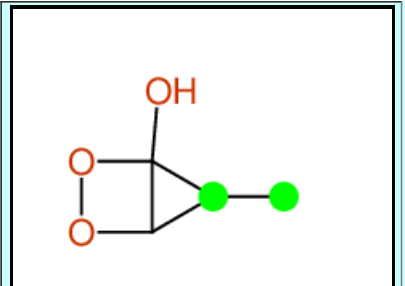
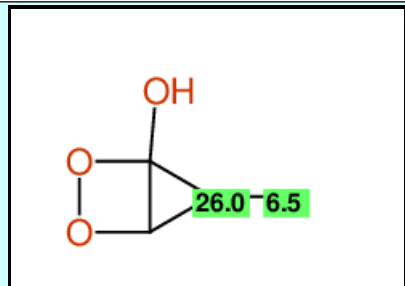


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### Structure Proposal #4

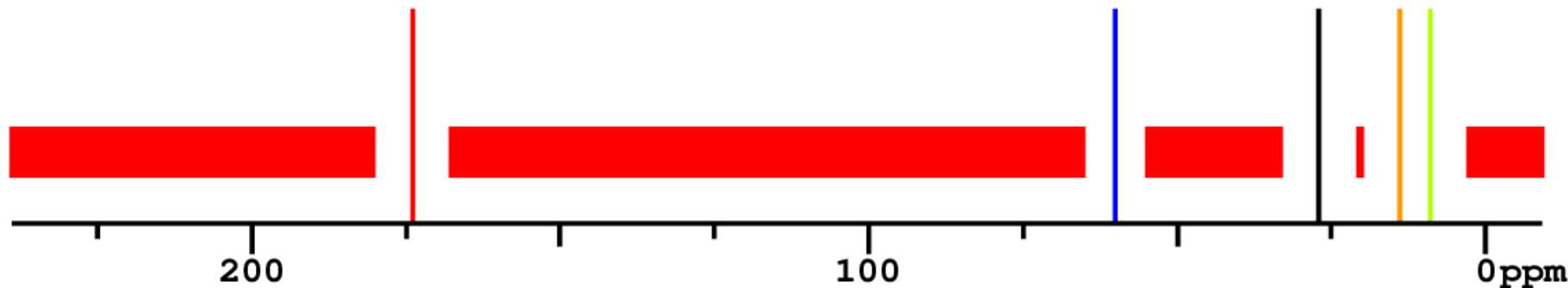
Structure	Similarity Measure
 <p>The chemical structure shows a bicyclic system consisting of a four-membered ring fused to a five-membered ring. The four-membered ring contains two oxygen atoms. The five-membered ring has a hydroxyl group (-OH) attached to one of its carbons. The overall structure is a bicyclic ether with a hydroxyl group.</p>	<p>Deviation = 3.94 ppm Similarity = 100 %</p> <p><math>C_4H_6O_3</math></p> <p>MWT = 102.04</p> <p>Search Web for this structure: <a href="#">JGBLVVQAZJCZED</a></p>
Predicted Chemical Shiftvalues	Matching Map





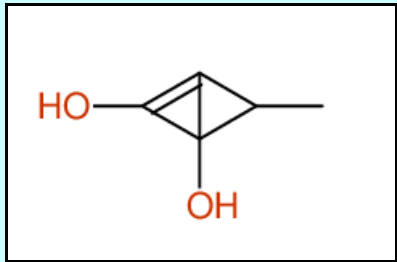
Experimental shift values

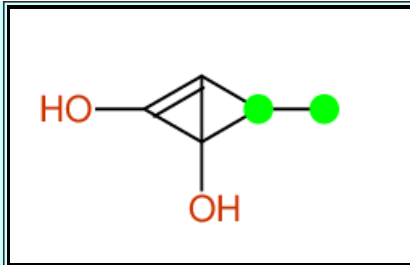
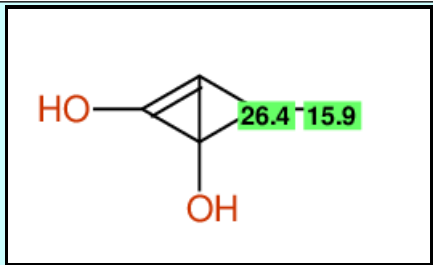
No line in reference: 



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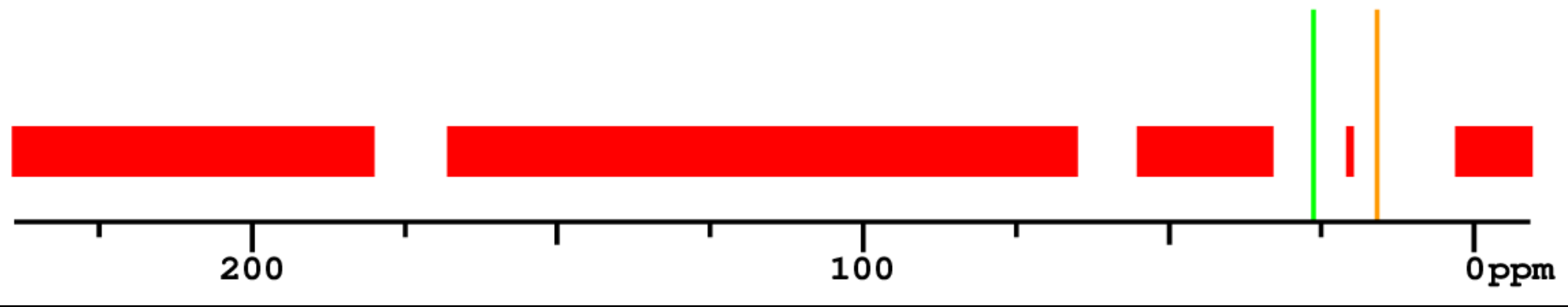
### Structure Proposal #5

Structure	Similarity Measure
	Deviation = 4.24 ppm Similarity = 100 %  $C_5H_6O_2$  MWT = 98.06 Search Web for this structure: <a href="#">YLSGXAZACMXQK</a>
Predicted Chemical Shiftvalues	Matching Map




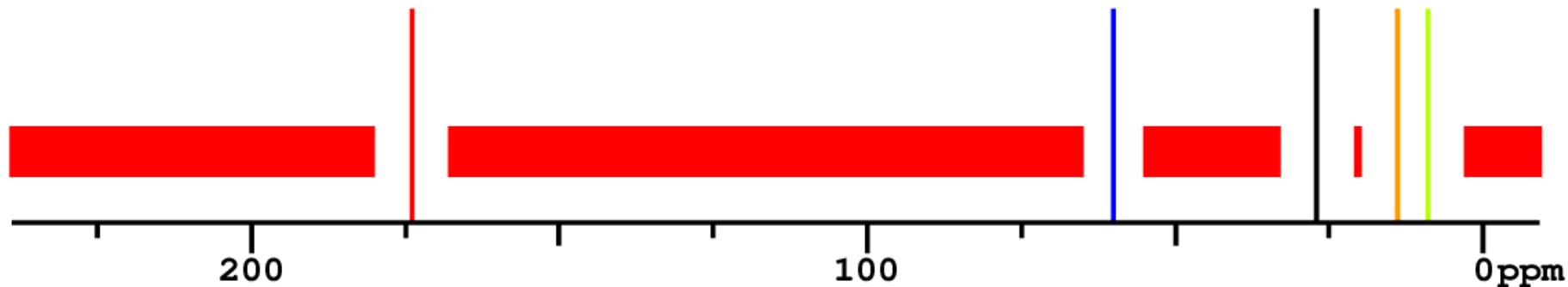
Predicted shift values

Signal multiplicity: S D T Q O E P ?



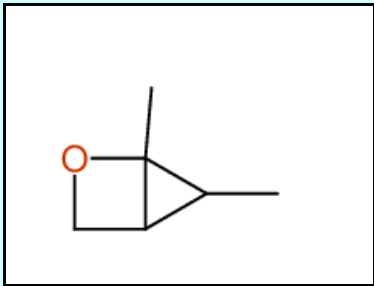
Experimental shift values

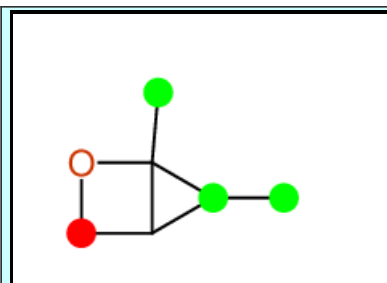
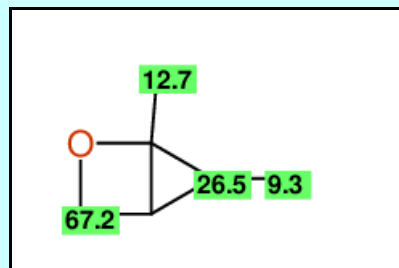
No line in reference: 



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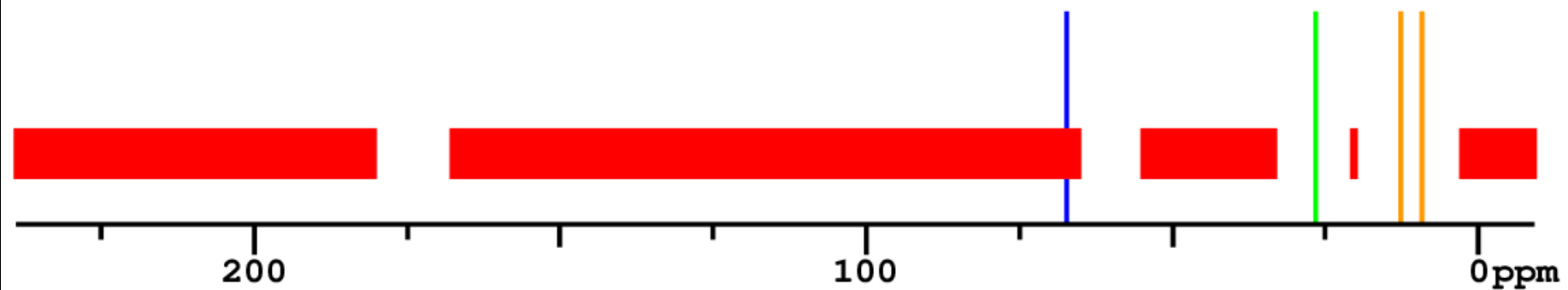
### Structure Proposal #6

Structure	Similarity Measure
	<p>Deviation = 4.28 ppm Similarity = 75 % (Different pattern)</p> <p><math>C_6H_{10}O</math></p> <p>MWT = 98.07</p> <p>Search Web for this structure: <a href="#">RRUPDGSLWBNUSW</a></p>
Predicted Chemical Shiftvalues	Matching Map



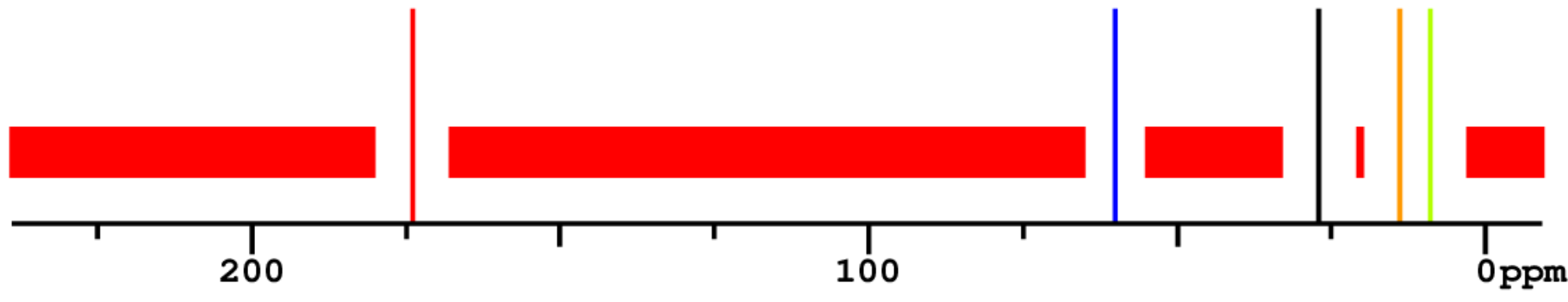
Predicted shift values

Signal multiplicity: S D T Q O E P ?



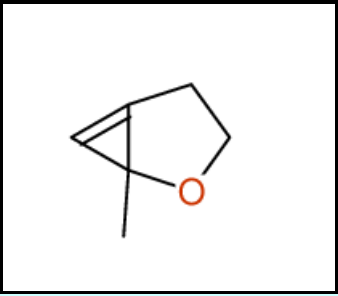
Experimental shift values

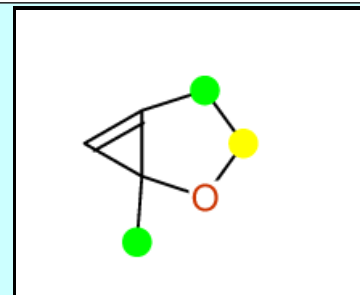
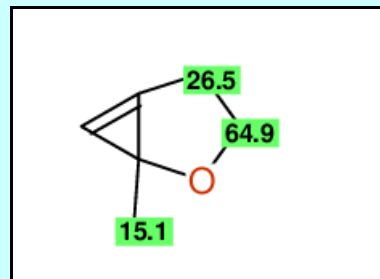
No line in reference: 



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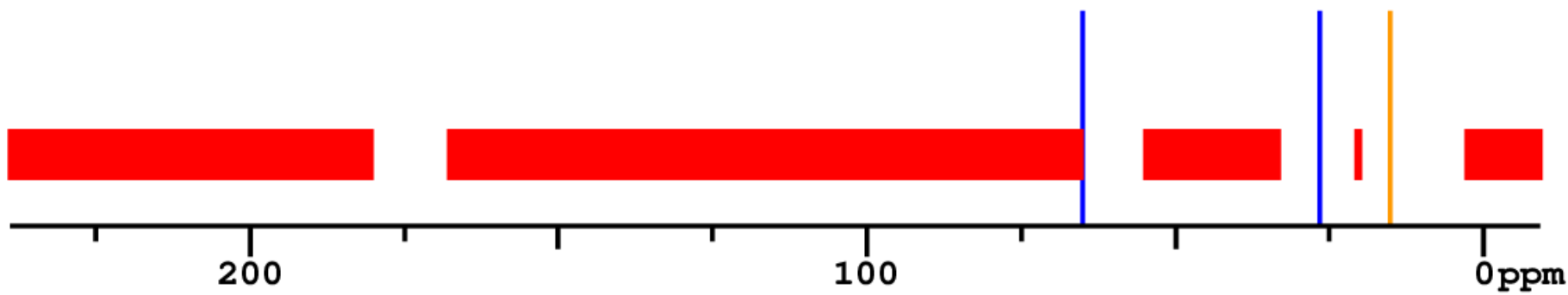
Structure Proposal #7

Structure	Similarity Measure
	Deviation = 4.46 ppm Similarity = 83 %  C <sub>6</sub> H <sub>8</sub> O  MWT = 96.07  Search Web for this structure:  <a href="#">MLKQXIPGHOLEQI</a>
Predicted Chemical Shiftvalues	Matching Map



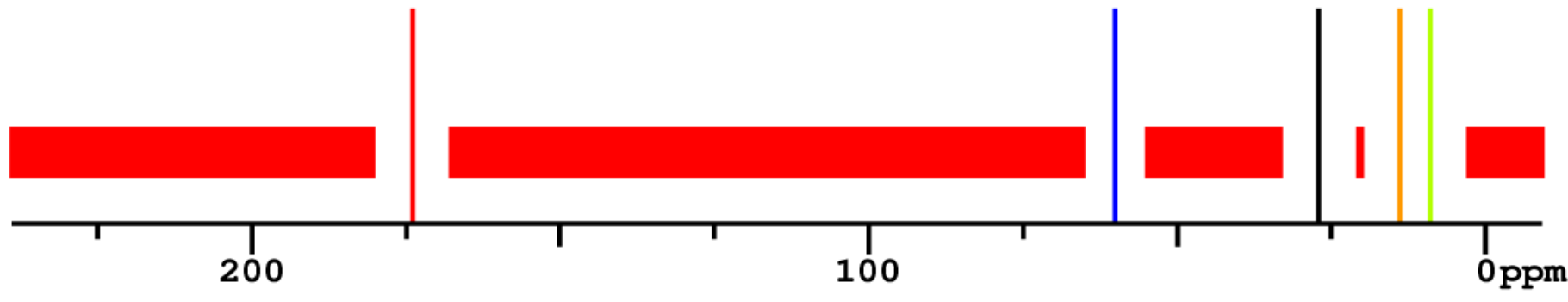
Predicted shift values

Signal multiplicity: S D T Q O E P ?



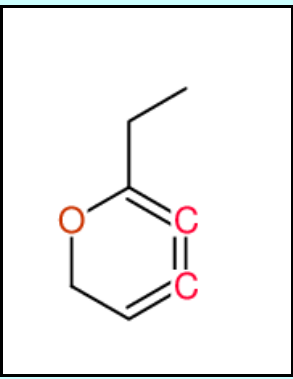
Experimental shift values

No line in reference: 

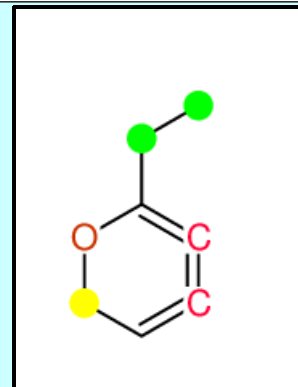
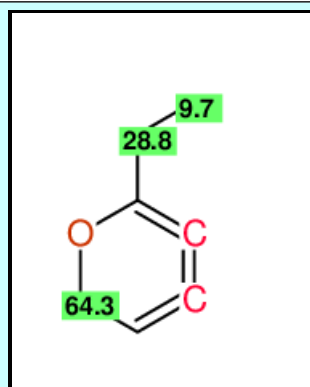


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### Structure Proposal #8

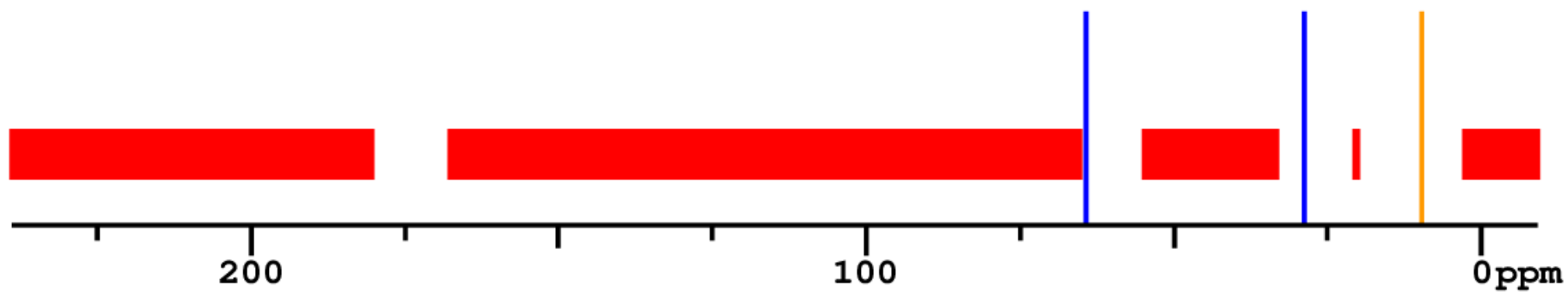
Structure	Similarity Measure
	Deviation = 4.60 ppm Similarity = 83 %  C <sub>7</sub> H <sub>8</sub> O  MWT = 108.08  Search Web for this structure: <a href="#">PNZSQYMQDYDJ</a>
Predicted Chemical Shiftvalues	Matching Map





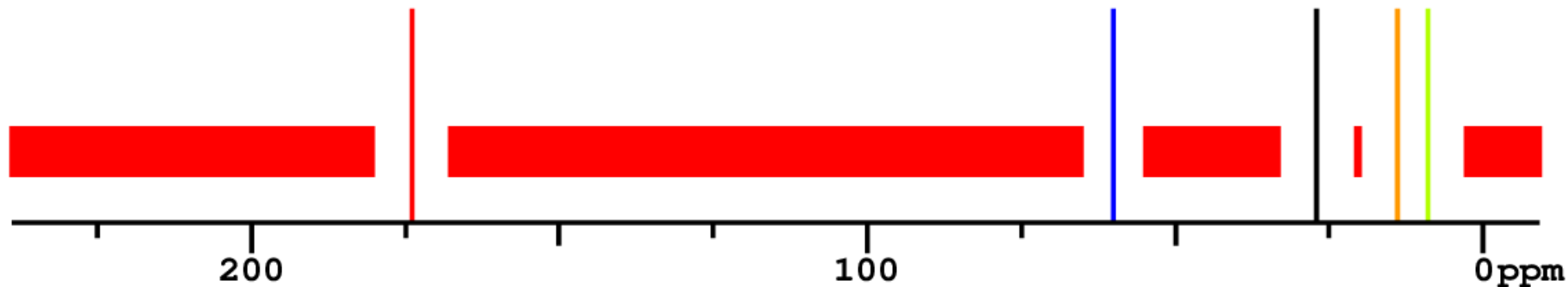
Predicted shift values

Signal multiplicity: S D T Q O E P ?



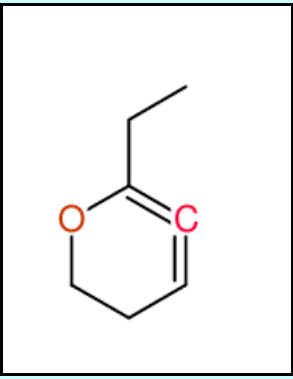
Experimental shift values

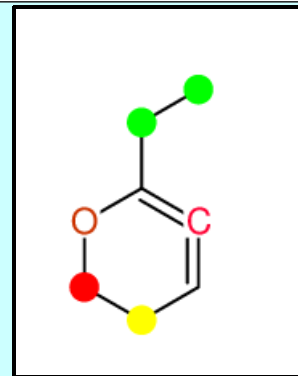
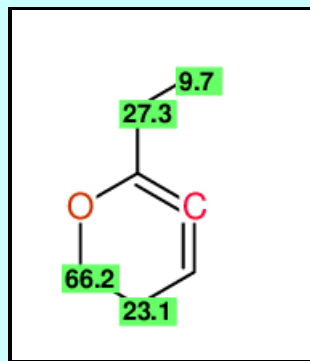
No line in reference: ████████



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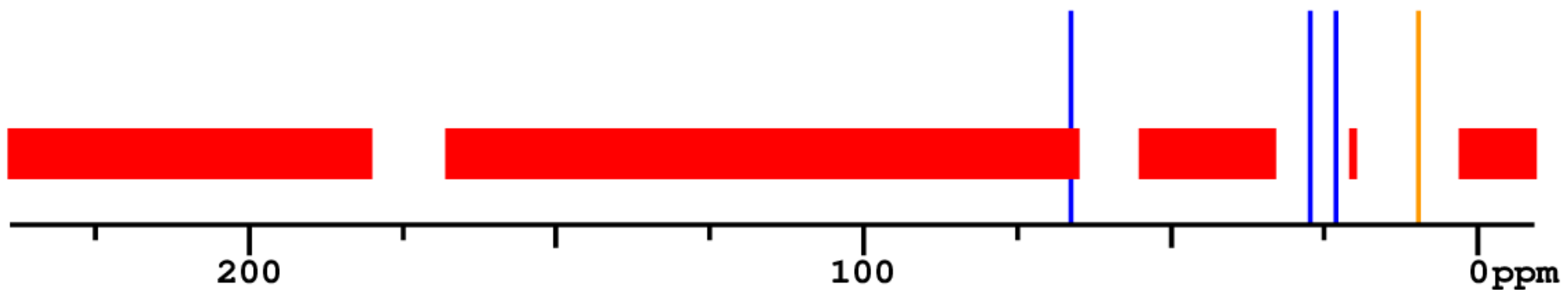
### Structure Proposal #9

Structure	Similarity Measure
	<p>Deviation = 4.70 ppm Similarity = 63 % (Different pattern)</p> <p><math>C_7H_{10}O</math></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">DRDGAMGKENXWCN</a></p>
Predicted Chemical Shiftvalues	Matching Map



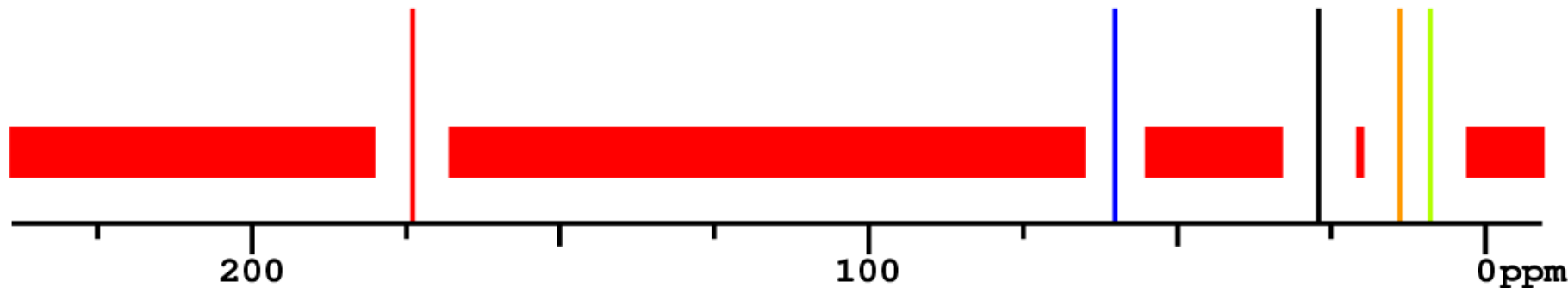
Predicted shift values

Signal multiplicity: S D T Q O E P ?



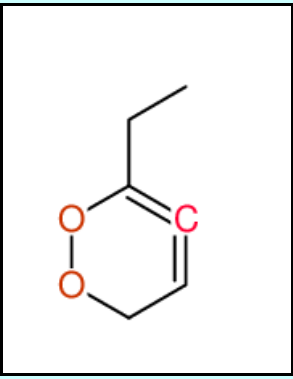
Experimental shift values

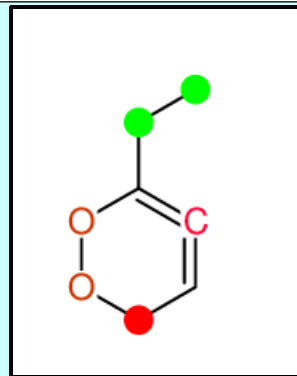
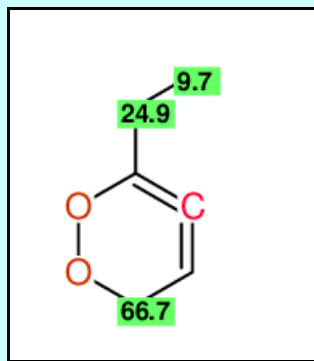
No line in reference: 



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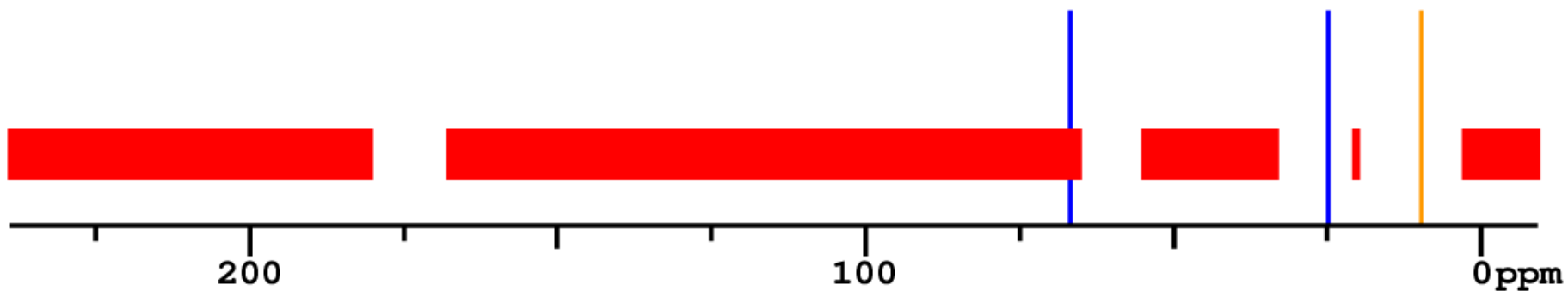
### Structure Proposal #10

Structure	Similarity Measure
	<p>Deviation = 4.72 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_8O_2</math></p> <p>MWT = 112.07</p> <p>Search Web for this structure: <a href="#">HQZWXOPRWOPVAU</a></p>
Predicted Chemical Shiftvalues	Matching Map



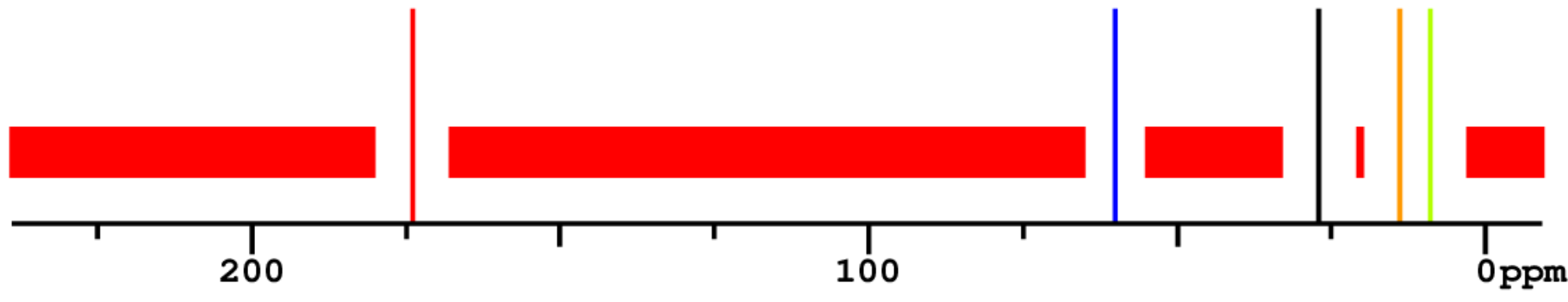
Predicted shift values

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



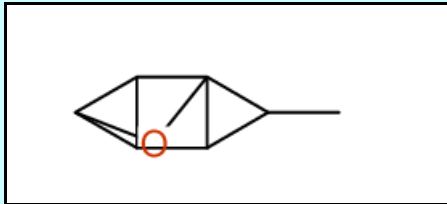
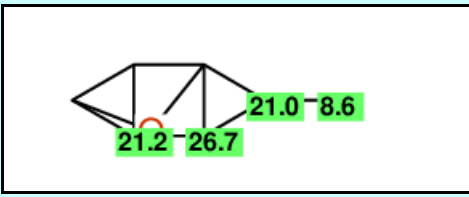
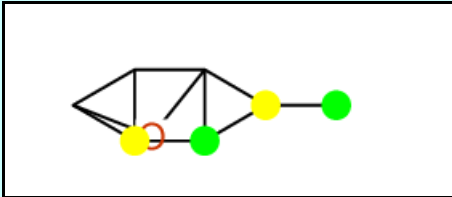
Experimental shift values

No line in reference: 



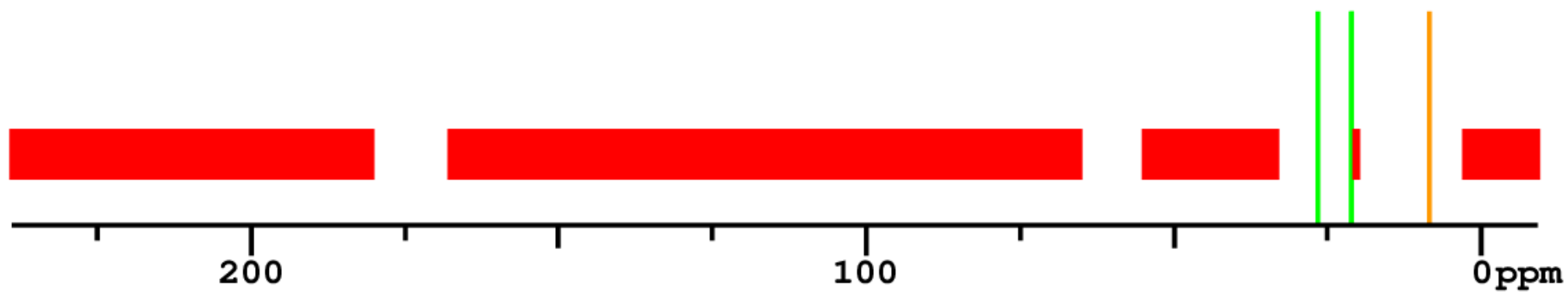
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### Structure Proposal #11

Structure	Similarity Measure
	Deviation = 4.78 ppm Similarity = 75 %  C <sub>7</sub> H <sub>8</sub> O  MWT = 108.08  Search Web for this structure:  <a href="#">RPKFKSYMKPKZHO</a>
Predicted Chemical Shiftvalues	Matching Map
	

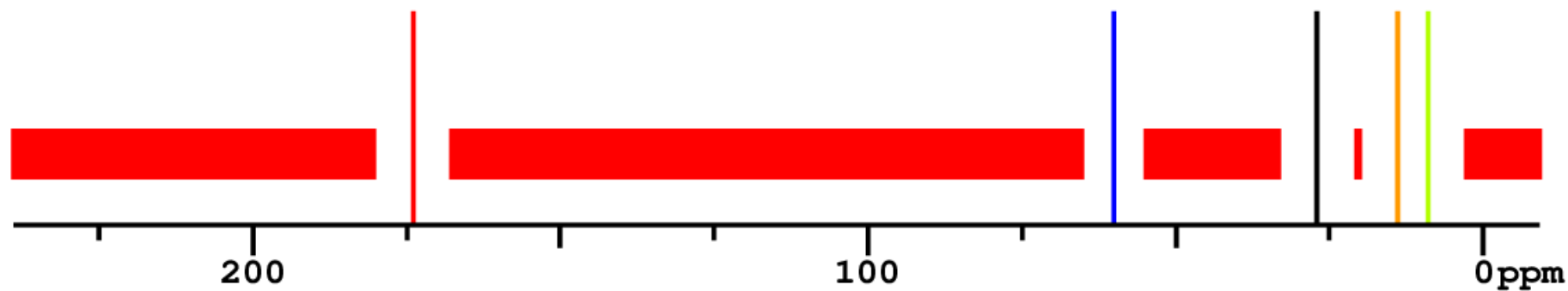
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

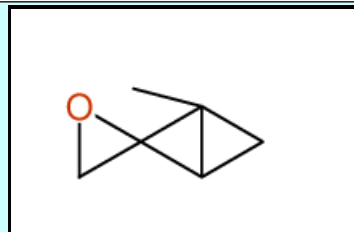
No line in reference: [red bar]



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### Structure Proposal #12

Structure	Similarity Measure
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Deviation = 4.90 ppm  
Similarity = 100 %

$C_6H_8O$

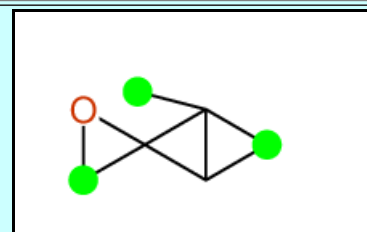
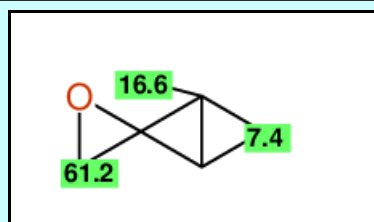
MWT = 96.07

Search Web for this  
structure:

[LOABURPYMMQUIT](#)

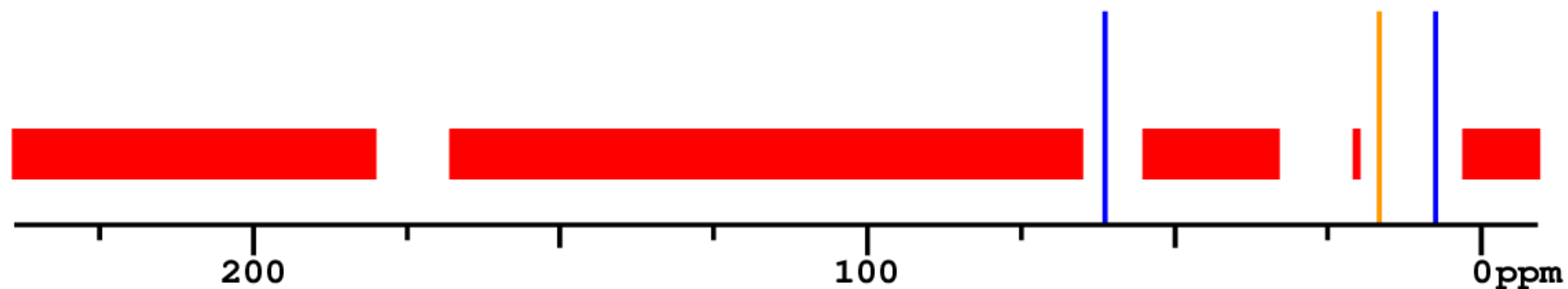
Predicted Chemical  
Shiftvalues

Matching Map



Predicted shift values

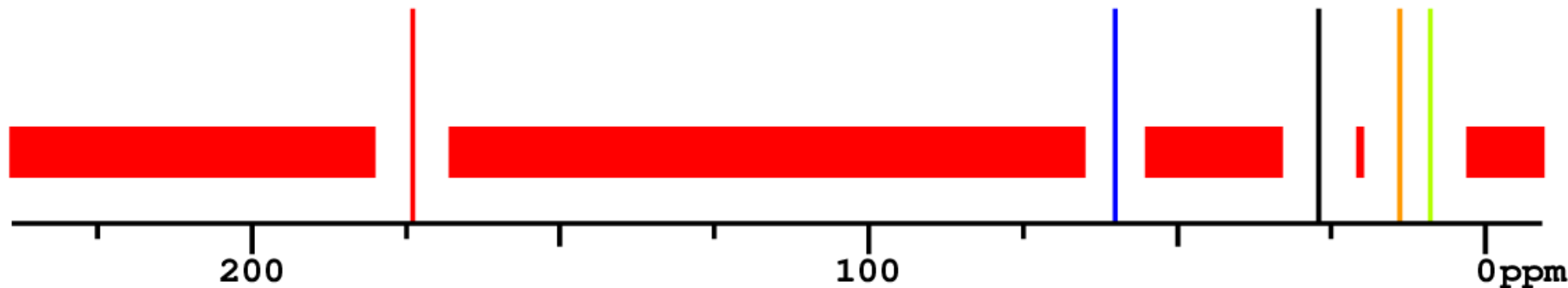
Signal multiplicity: **S****D****T****Q****O****E****P**?





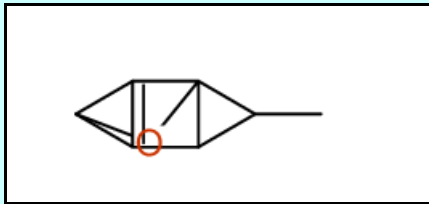
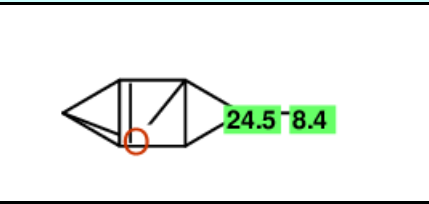
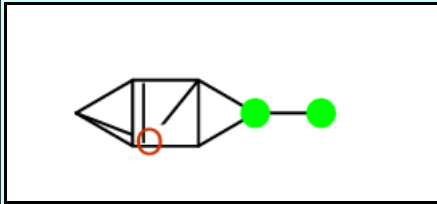
Experimental shift values

No line in reference: 



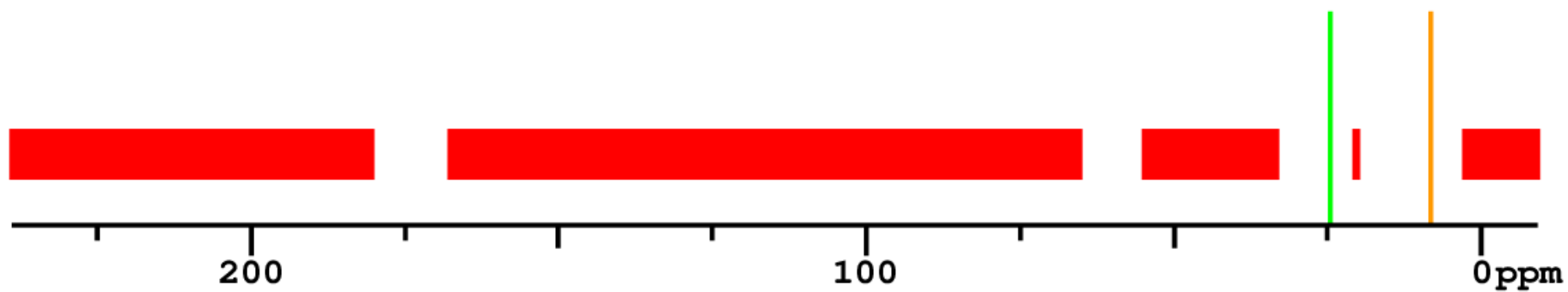
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### Structure Proposal #13

Structure	Similarity Measure
	Deviation = 5.10 ppm Similarity = 100 %  C <sub>7</sub> H <sub>6</sub> O  MWT = 106.08  Search Web for this structure:  <a href="#">HDESMDVUQOYCMC</a>
Predicted Chemical Shiftvalues	Matching Map
	

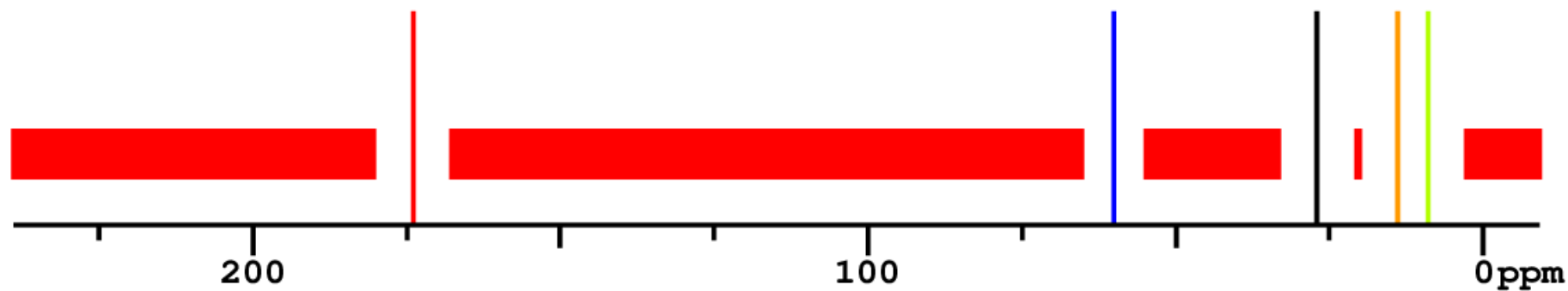
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

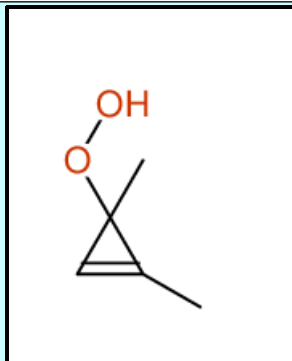
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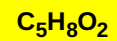
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### Structure Proposal #14

Structure	Similarity Measure



Deviation = 5.12 ppm  
Similarity = 100 %



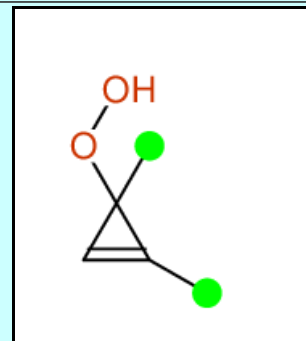
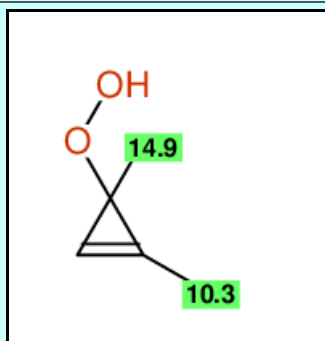
MWT = 100.06

Search Web for this  
structure:

[QJMTQIRFXBQEU](https://www.qjmtqirfxbqeu.com)

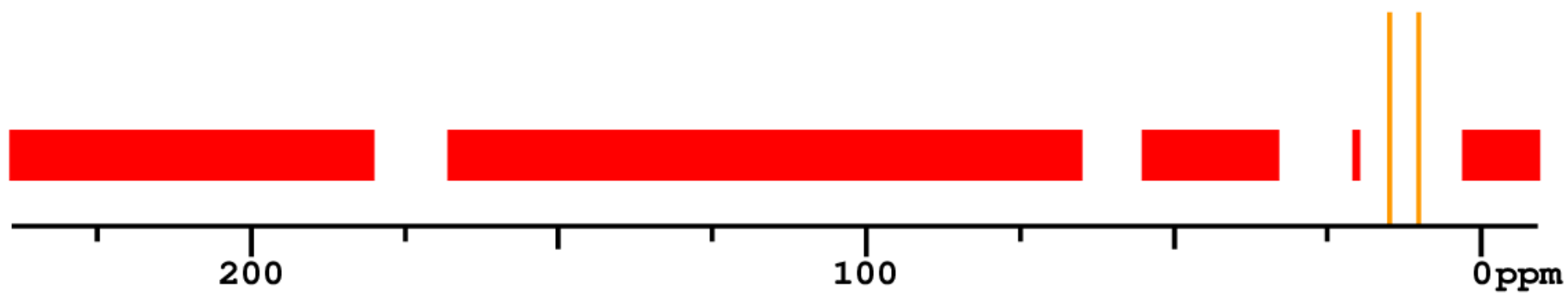
Predicted Chemical  
Shiftvalues

Matching Map



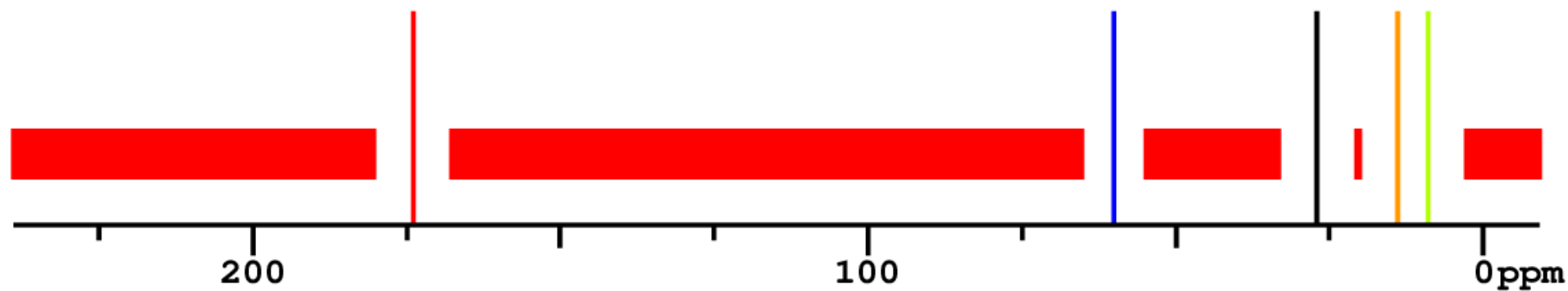
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

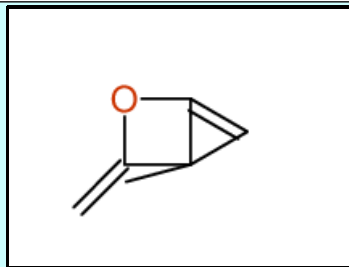
No line in reference: [red bar]



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### Structure Proposal #15

Structure	Similarity Measure



Deviation = 5.87 ppm  
Similarity = 100 %

$C_6H_6O$

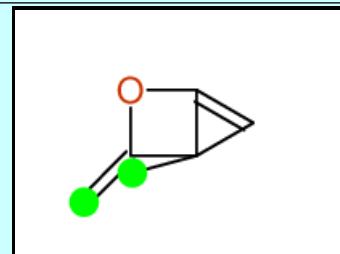
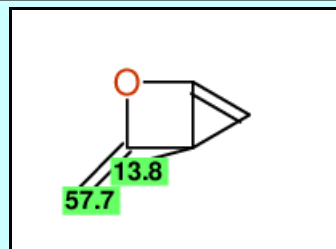
MWT = 94.07

Search Web for this  
structure:

[YDMXGLHNPWXWND](#)

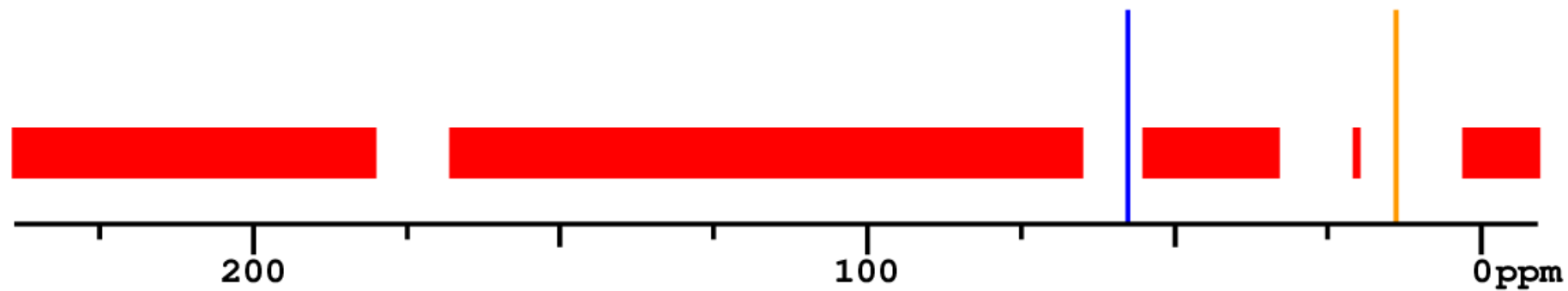
Predicted Chemical  
Shiftvalues

Matching Map




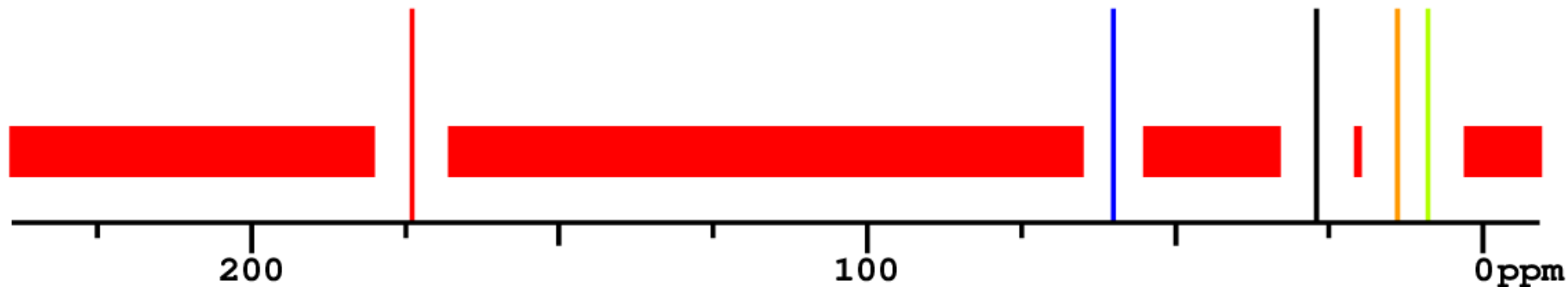
Predicted shift values

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



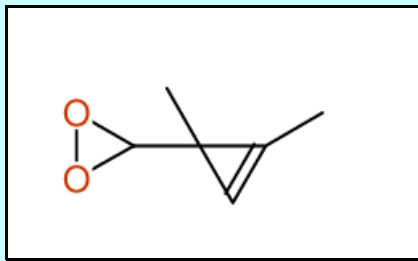
Experimental shift values

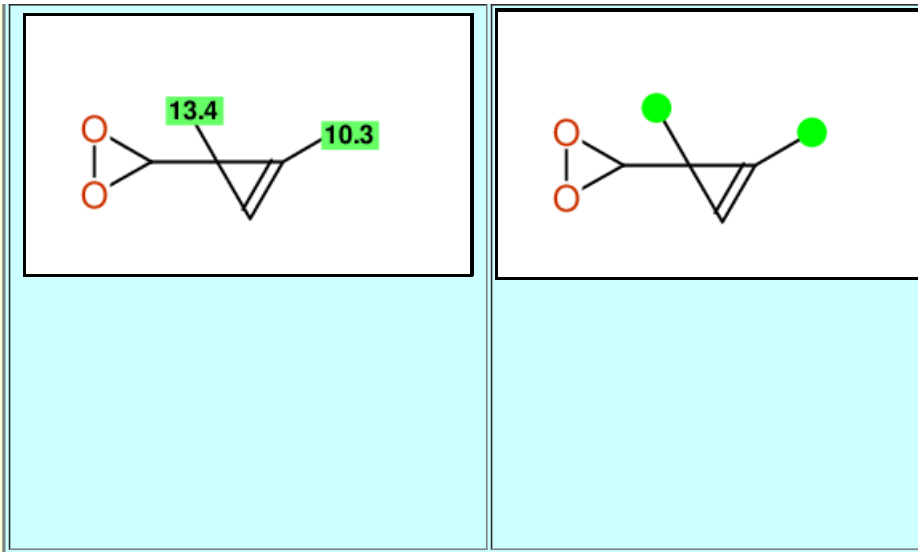
No line in reference: 



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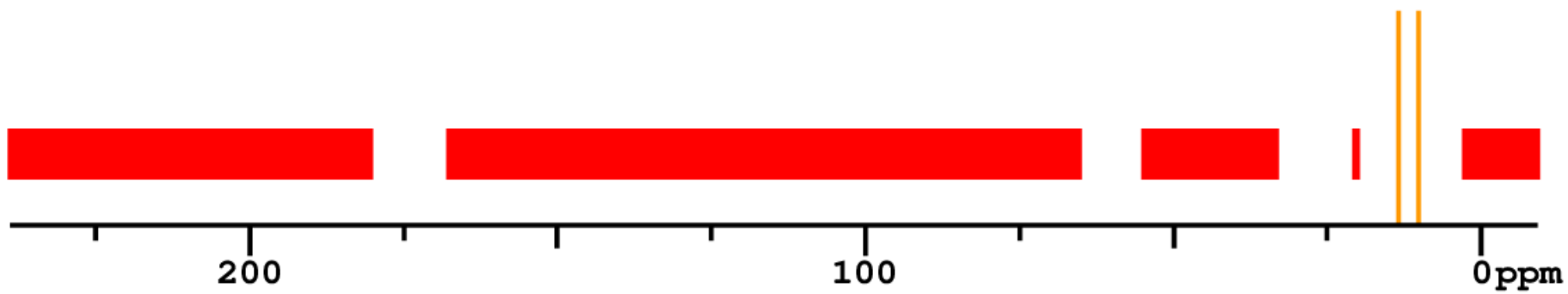
### Structure Proposal #16

Structure	Similarity Measure
	Deviation = 5.92 ppm Similarity = 100 %  $C_6H_8O_2$  MWT = 112.07 Search Web for this structure: <a href="#">AFXAYZSYHSLFGG</a>
Predicted Chemical Shiftvalues	Matching Map




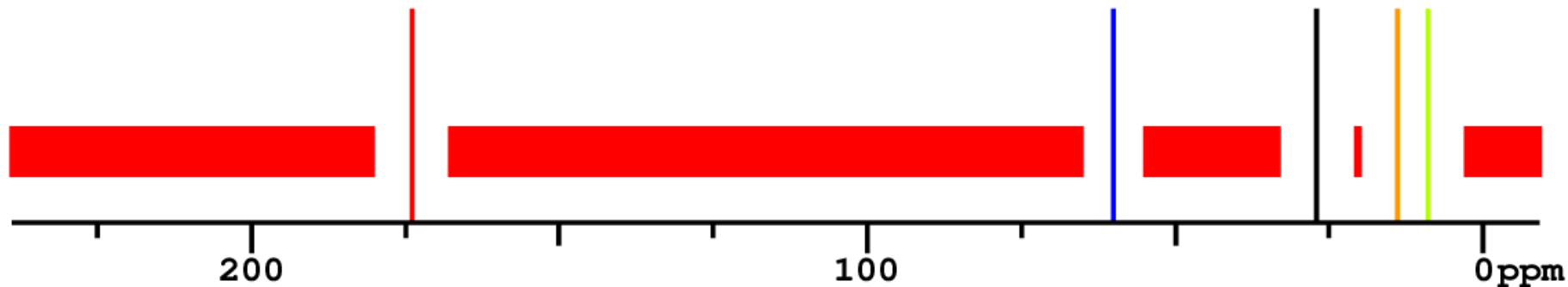
Predicted shift values

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



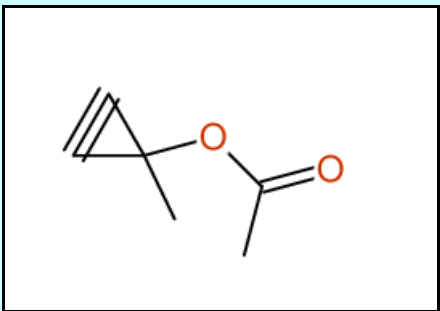
Experimental shift values

No line in reference: 

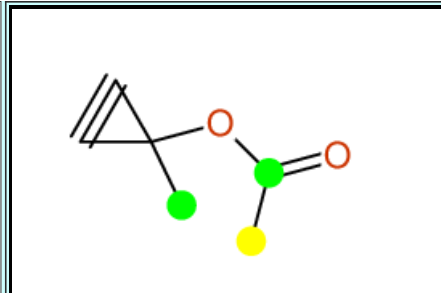
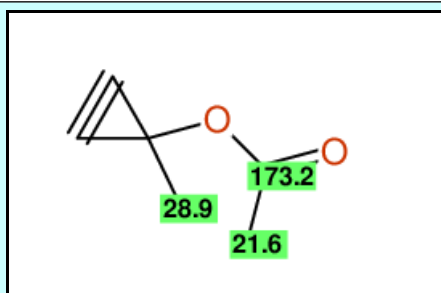


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### Structure Proposal #17

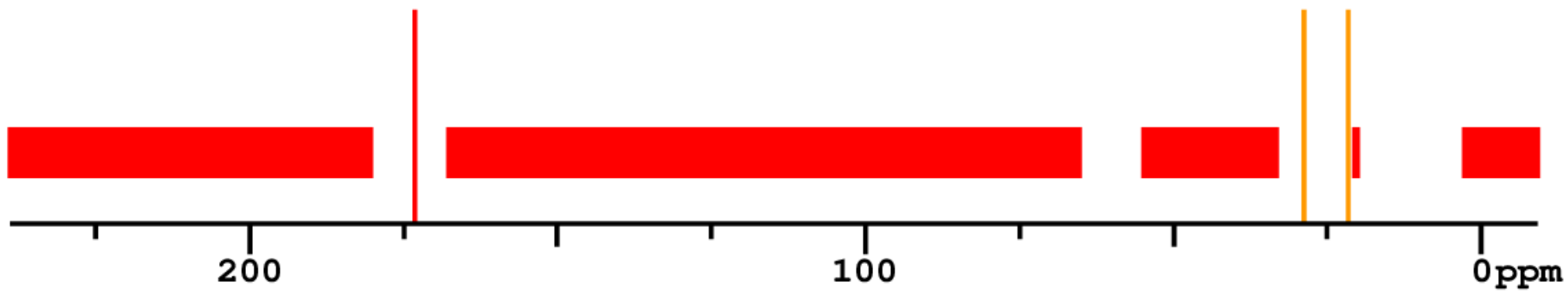
Structure	Similarity Measure
	Deviation = 5.94 ppm Similarity = 83 %  $C_6H_6O_2$  MWT = 110.07 Search Web for this structure: <a href="#">UBJMOXHHNZUDRL</a>
Predicted Chemical Shiftvalues	Matching Map





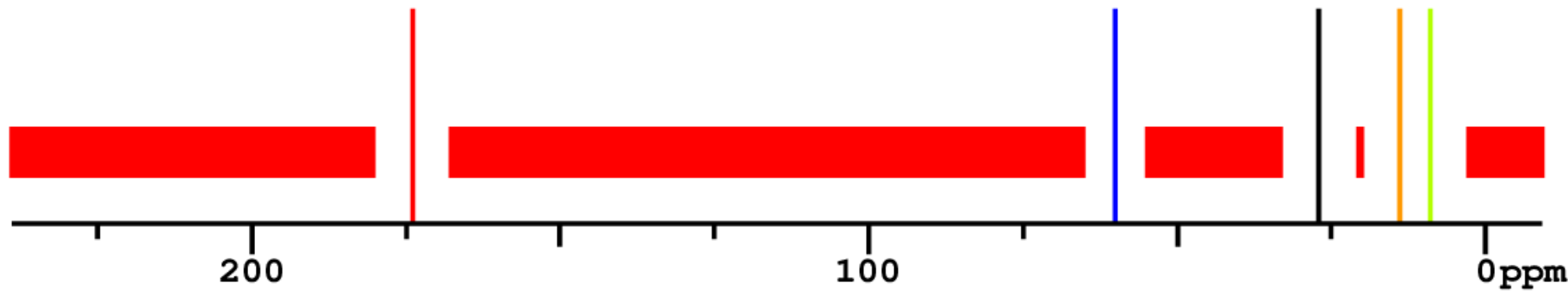
Predicted shift values

Signal multiplicity: S D T Q O E P ?



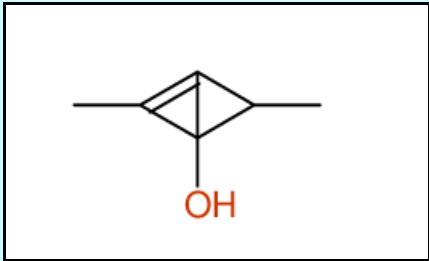
Experimental shift values

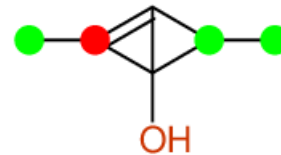
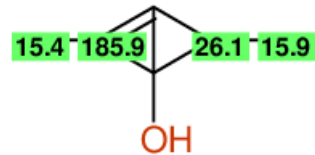
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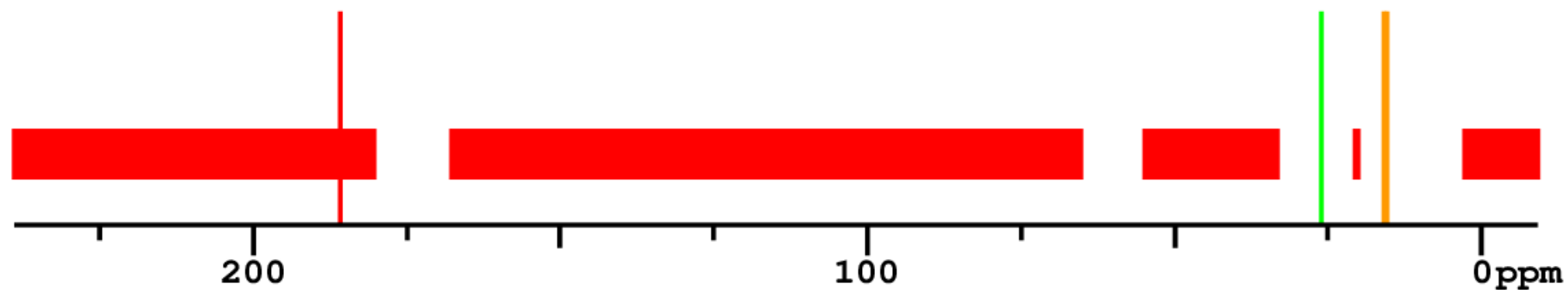
### Structure Proposal #18

Structure	Similarity Measure
	<p>Deviation = 6.26 ppm Similarity = 75 % (Different pattern)</p> <p><math>C_6H_8O</math></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">HEGRMNFFAOTRDL</a></p>
Predicted Chemical Shiftvalues	Matching Map



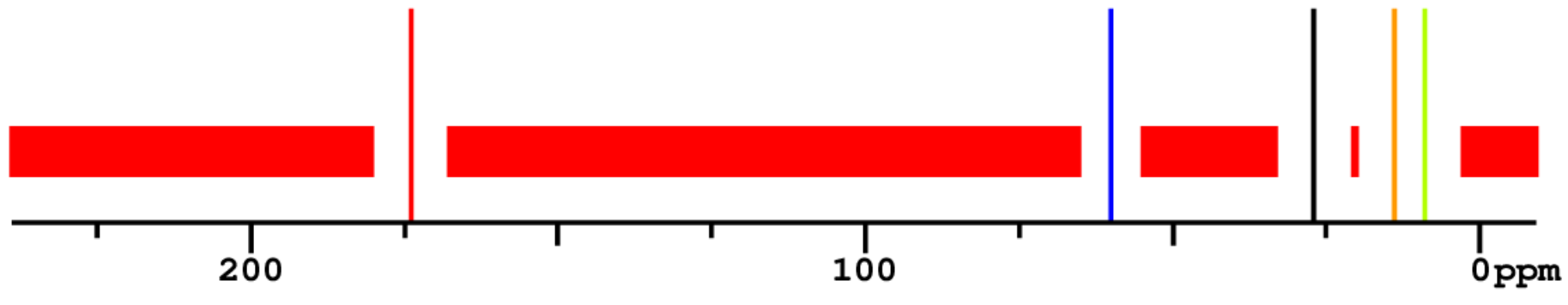
Predicted shift values

Signal multiplicity: S D T Q O E P ?



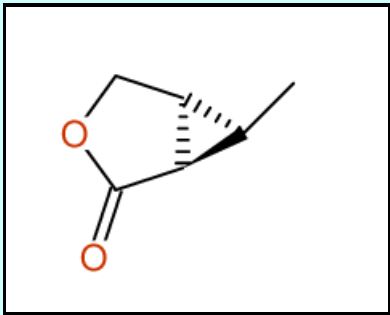
Experimental shift values

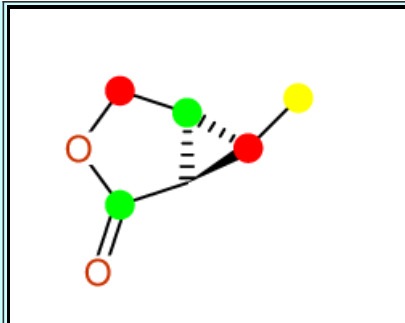
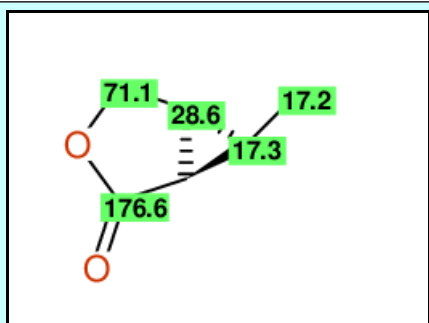
No line in reference: 



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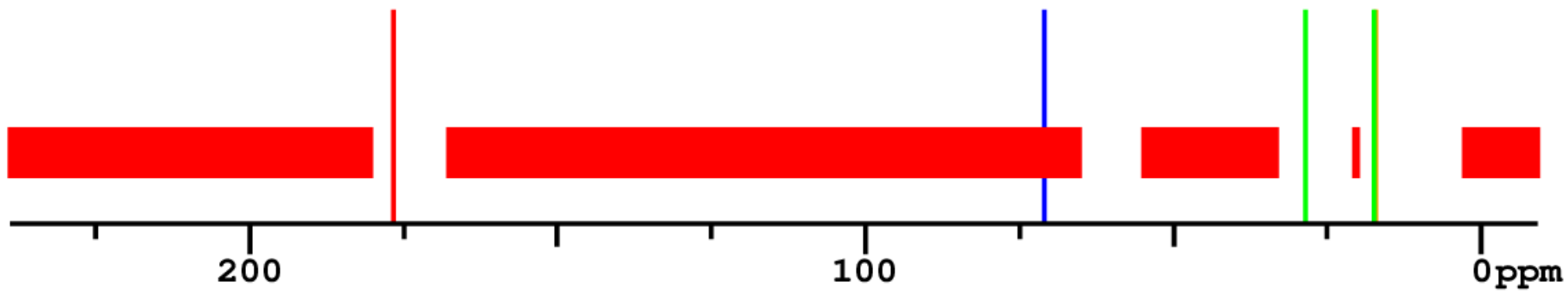
### Structure Proposal #19

Structure	Similarity Measure
	<p>Deviation = 6.45 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_6H_8O_2</math></p> <p>MWT = 112.07</p> <p>Search Web for this structure: <a href="#">ODZSNSOKRZBPDY</a></p>
Predicted Chemical Shiftvalues	Matching Map



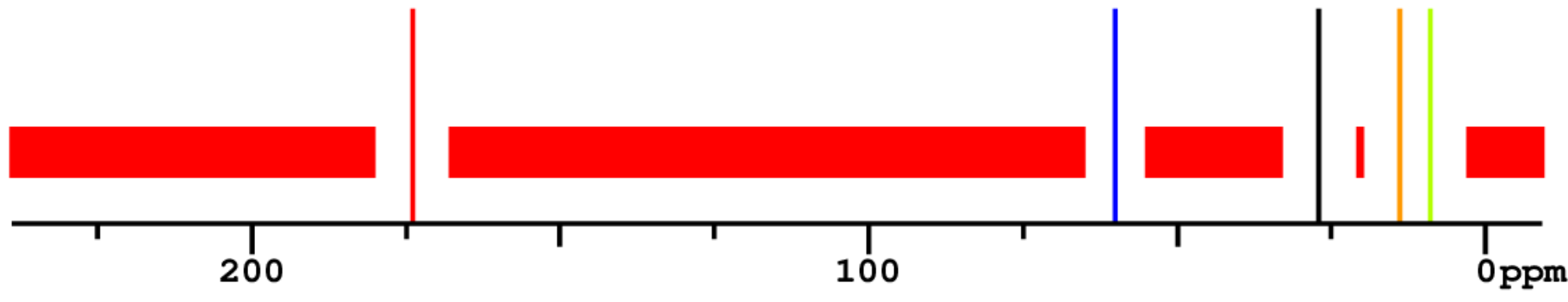
Predicted shift values

Signal multiplicity: S D T Q O E P ?



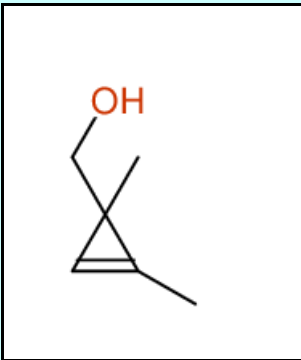
Experimental shift values

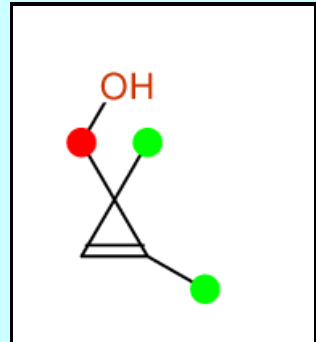
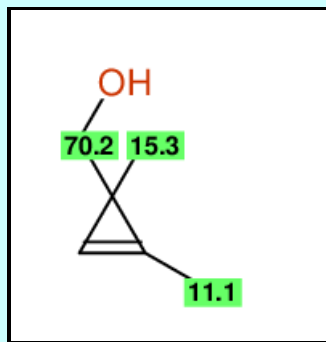
No line in reference: 



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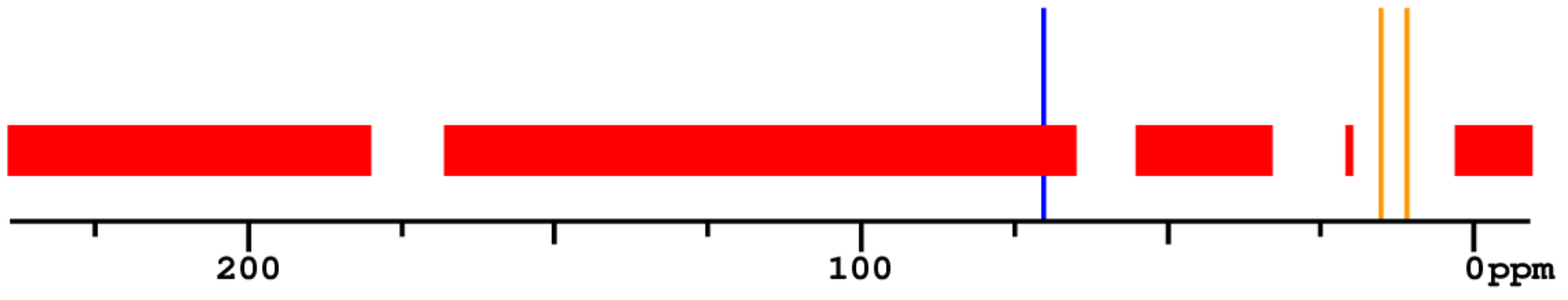
### Structure Proposal #20

Structure	Similarity Measure
	<p>Deviation = 6.70 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{10}O</math></p> <p>MWT = 98.07</p> <p>Search Web for this structure: <a href="#">XDZLYFBRUGYBSU</a></p>
Predicted Chemical Shiftvalues	Matching Map



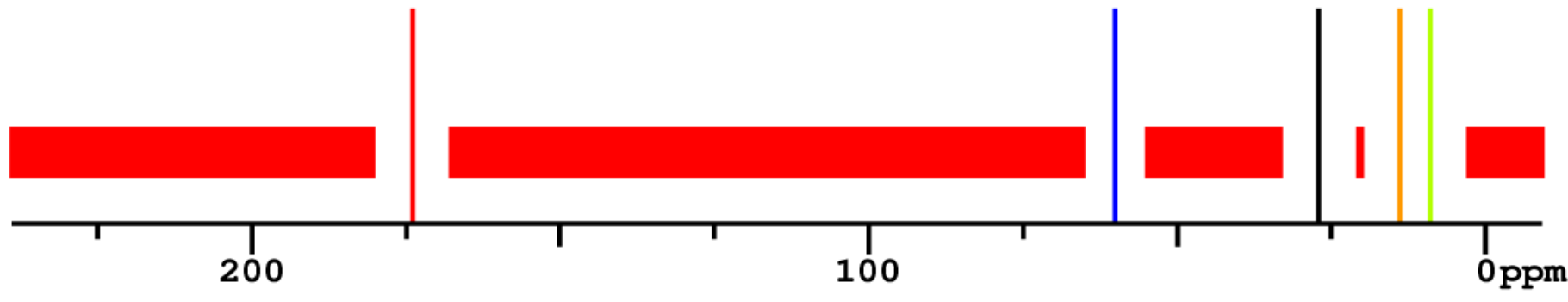
Predicted shift values

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



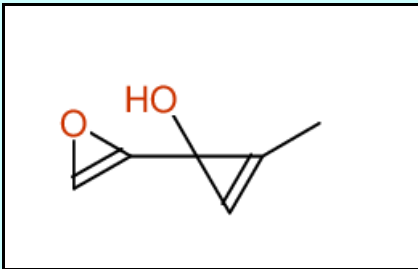
Experimental shift values

No line in reference: 

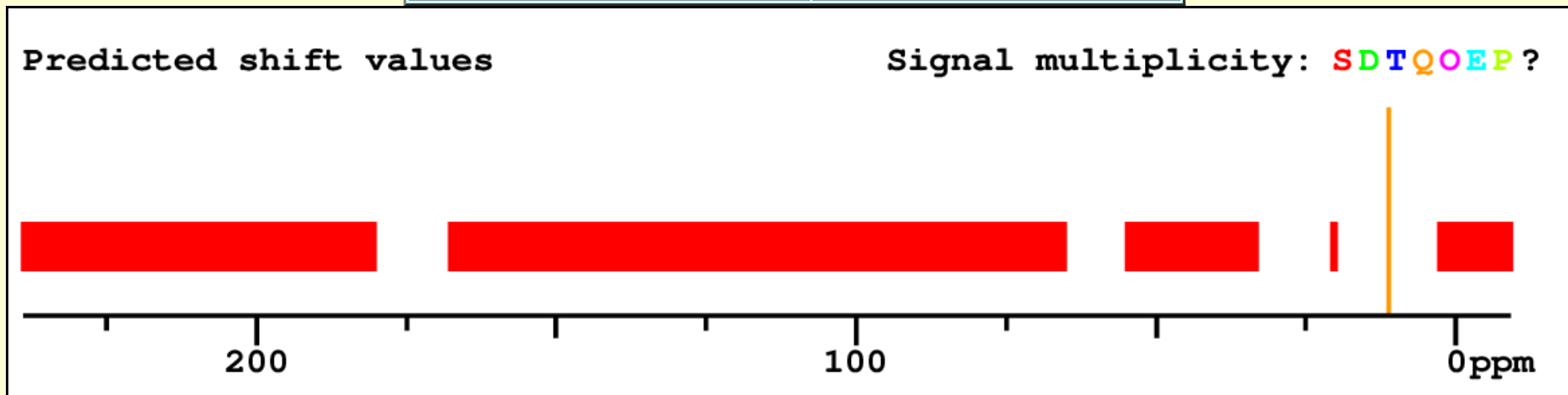
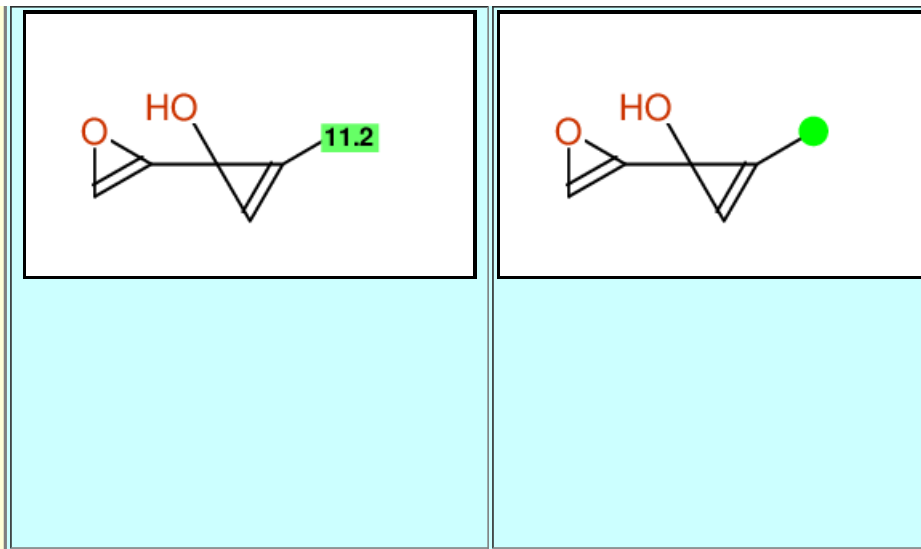


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### Structure Proposal #21

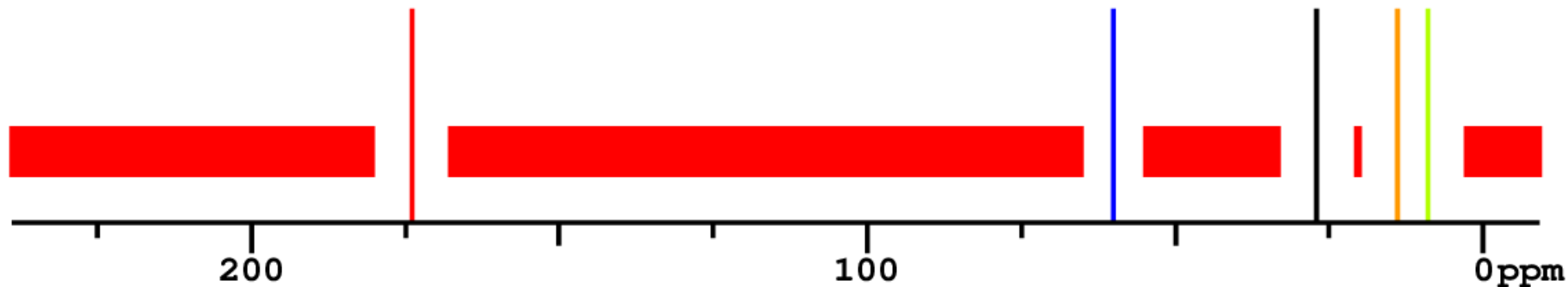
Structure	Similarity Measure
	Deviation = 6.73 ppm Similarity = 100 %  $C_6H_6O_2$  MWT = 110.07 Search Web for this structure: <a href="#">UMWSJQEYLPPQPB</a>
Predicted Chemical Shiftvalues	Matching Map





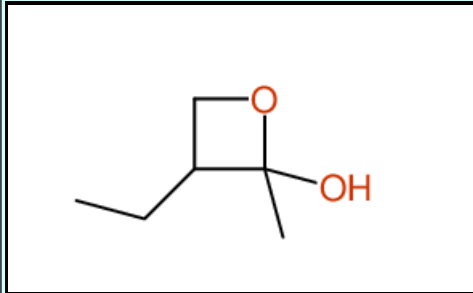
Experimental shift values

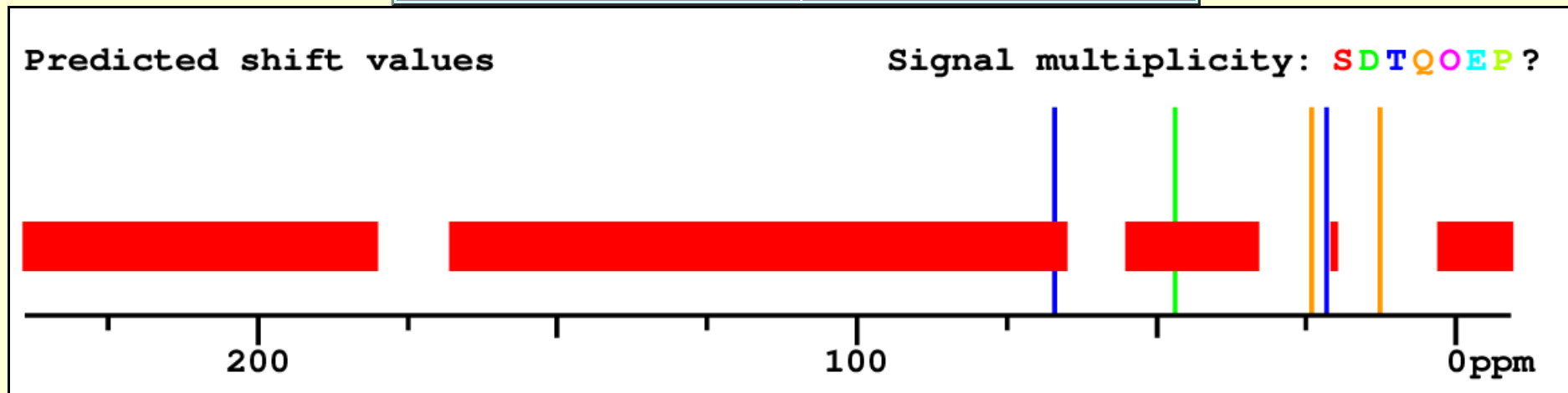
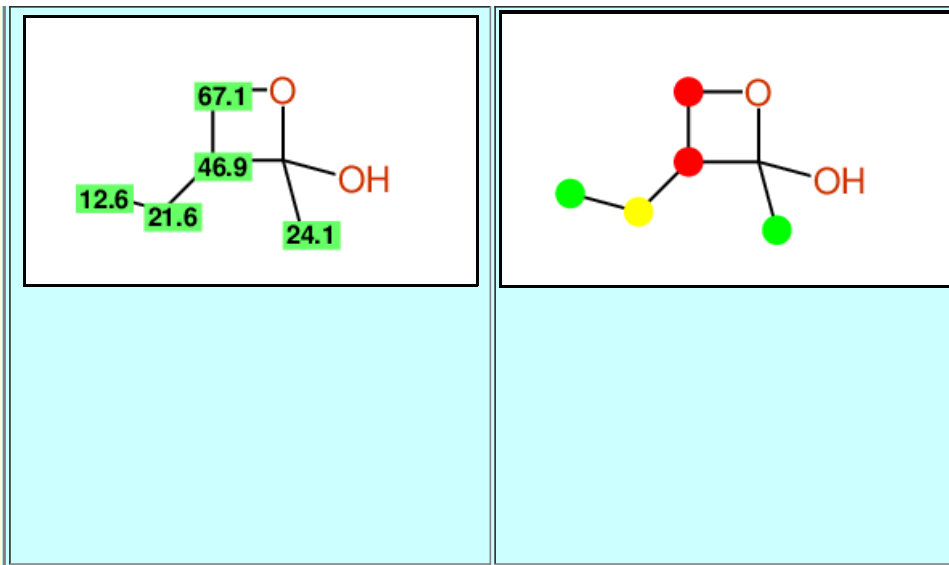
No line in reference: 



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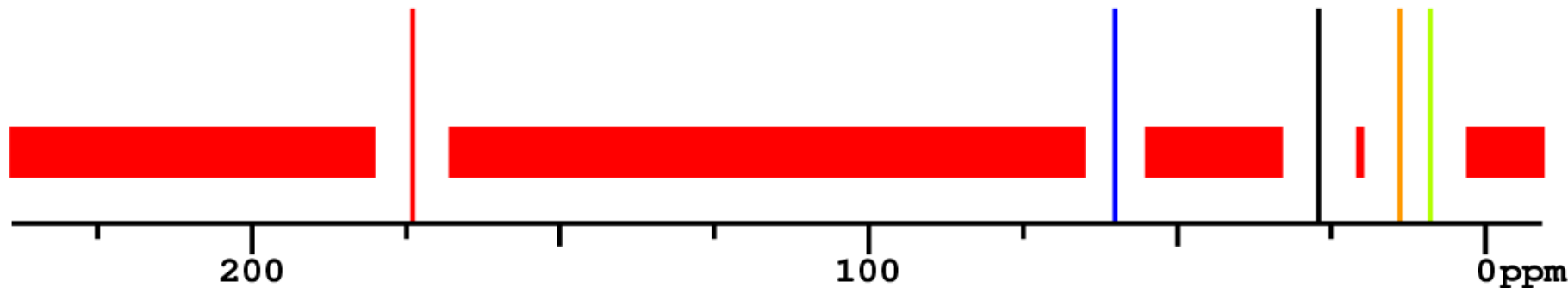
### Structure Proposal #22

Structure	Similarity Measure
	<p>Deviation = 6.89 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.07</p> <p>Search Web for this structure: <a href="#">DHCRDJAGJXWNRZ</a></p>
Predicted Chemical Shiftvalues	Matching Map



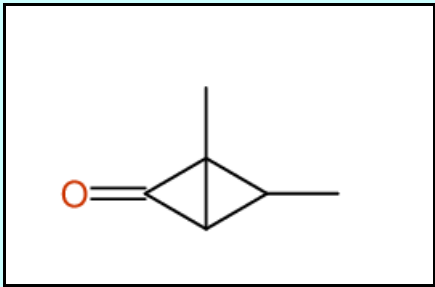
Experimental shift values

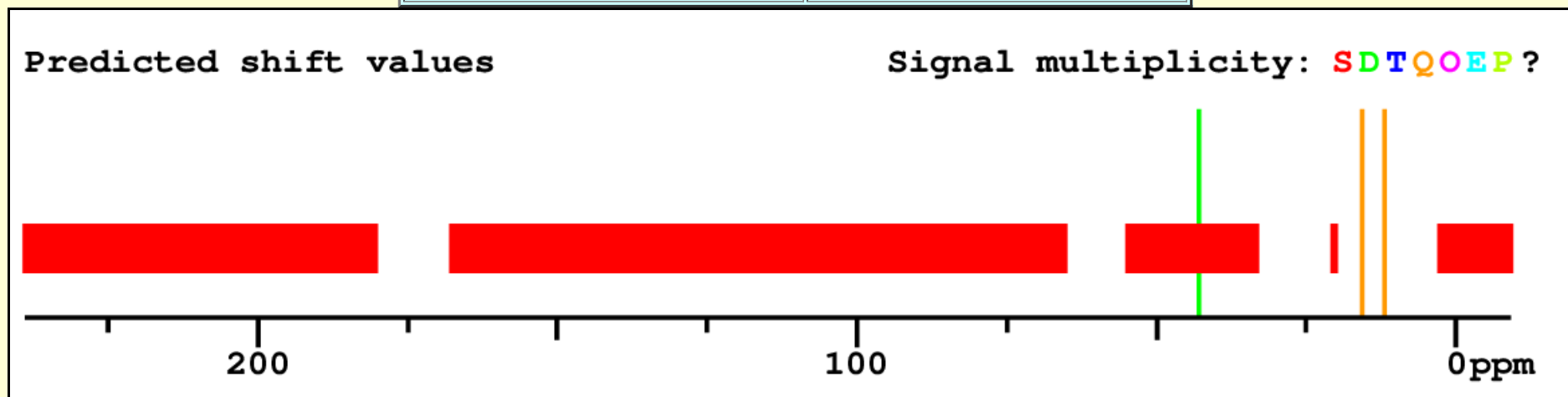
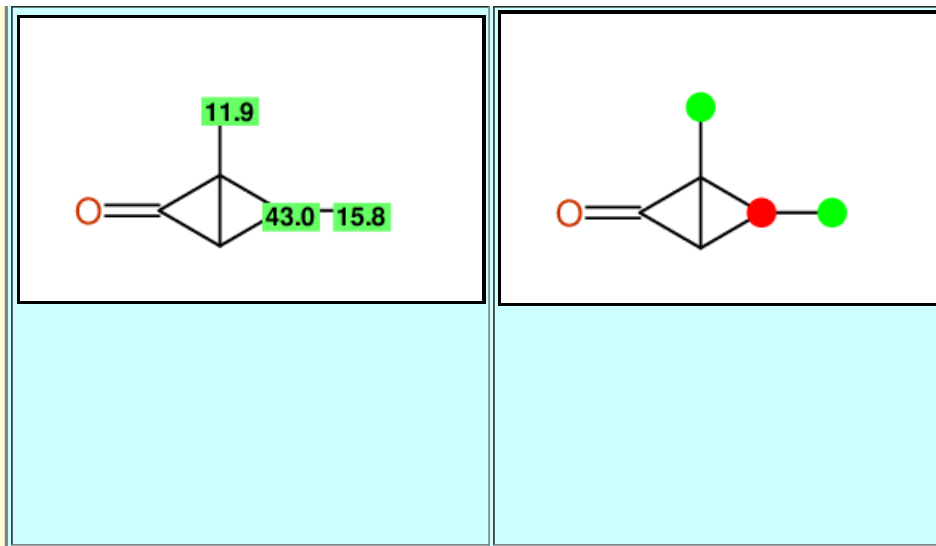
No line in reference: 



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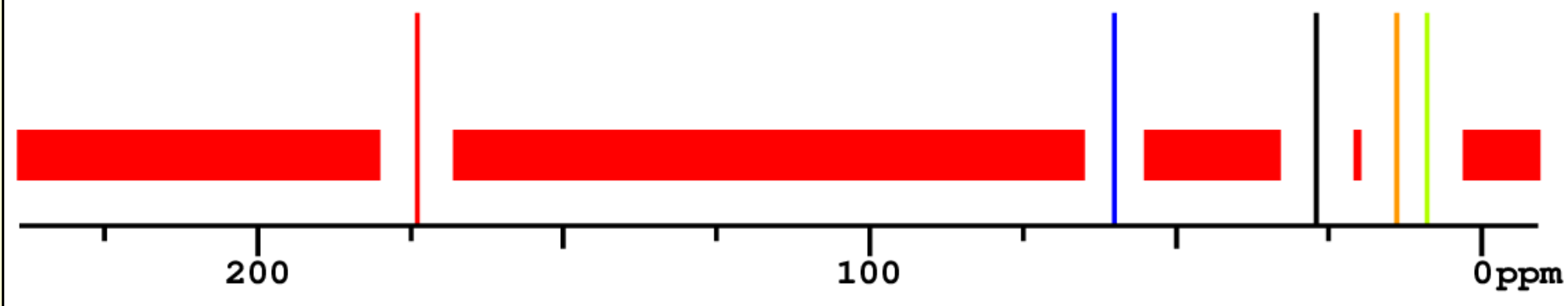
### Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 7.00 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_8O</math></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">SXZKEELVORMPAX</a></p>
Predicted Chemical Shiftvalues	Matching Map



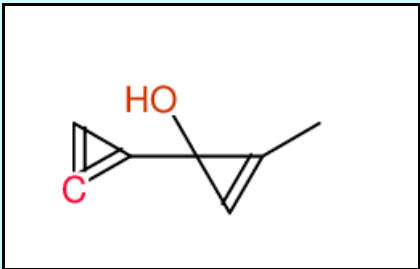
Experimental shift values

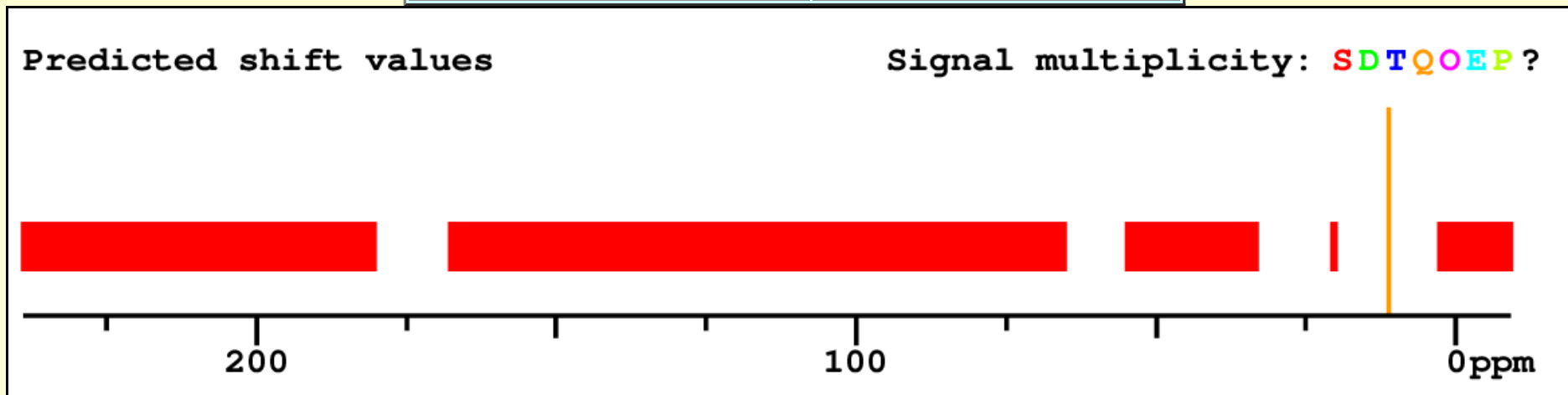
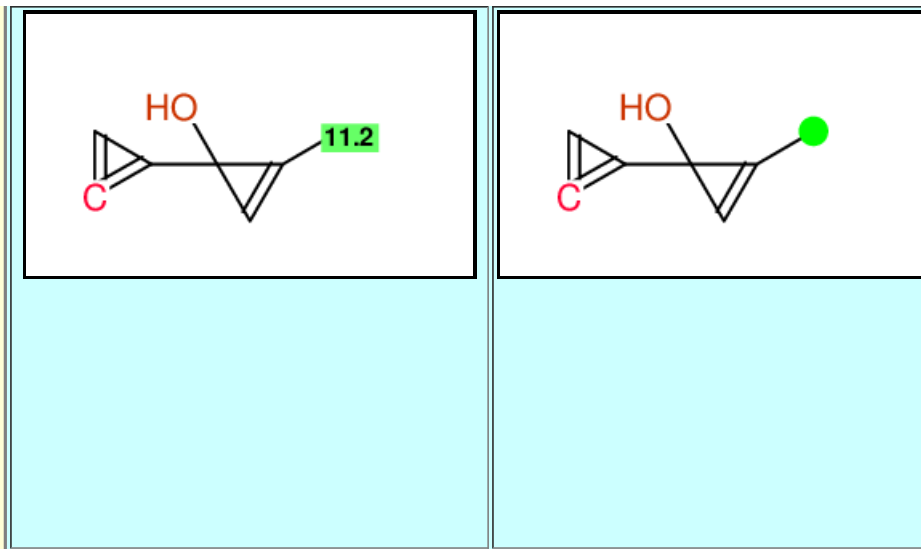
No line in reference: 



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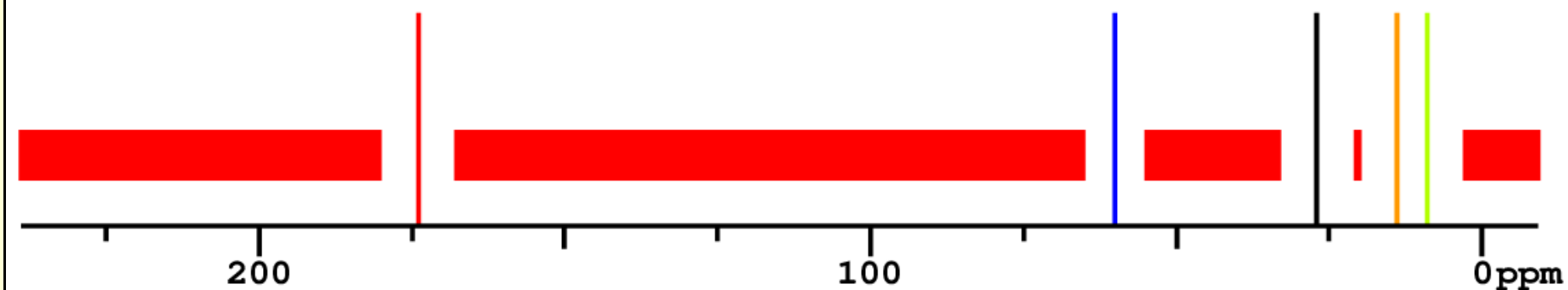
### Structure Proposal #24

Structure	Similarity Measure
 <p>The chemical structure shows a bicyclic system consisting of a cyclopropane ring fused to a cyclobutane ring. A hydroxyl group (HO) is attached to the cyclopropane ring, and a methyl group is attached to the cyclobutane ring. A carbon atom in the cyclopropane ring is highlighted in red and labeled 'C'.</p>	<p>Deviation = 7.22 ppm Similarity = 100 %</p> <p><math>C_7H_6O</math></p> <p>MWT = 106.08</p> <p>Search Web for this structure: <a href="#">PZRCSSMZNSBWQR</a></p>
Predicted Chemical Shiftvalues	Matching Map



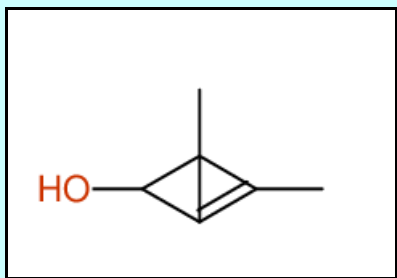
Experimental shift values

No line in reference: ████████

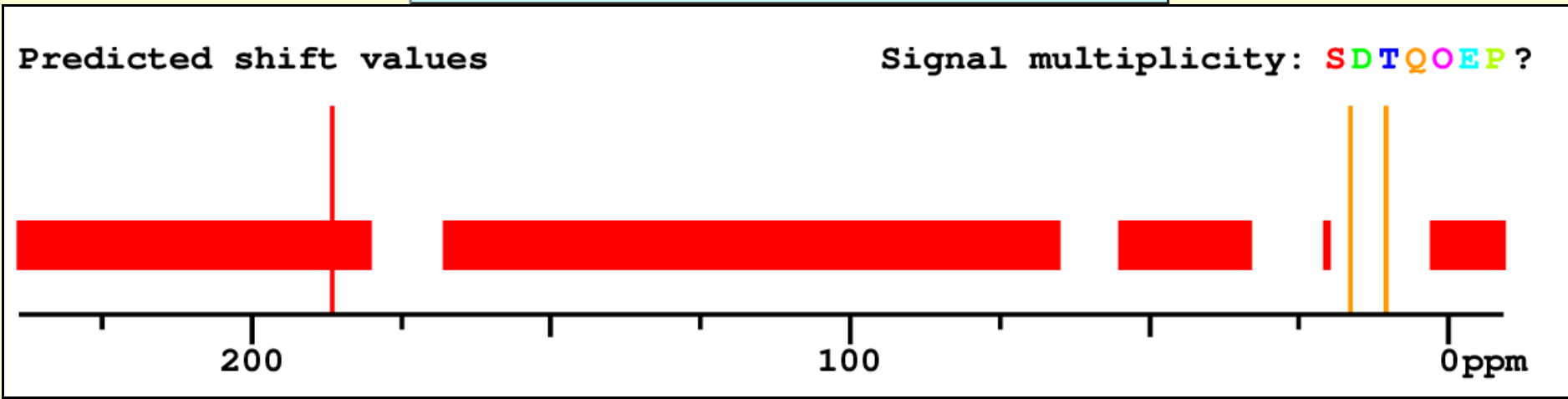
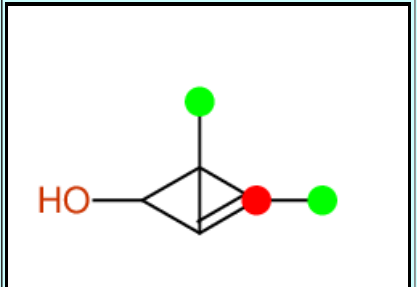
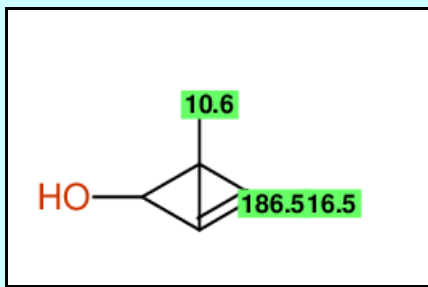


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### Structure Proposal #25

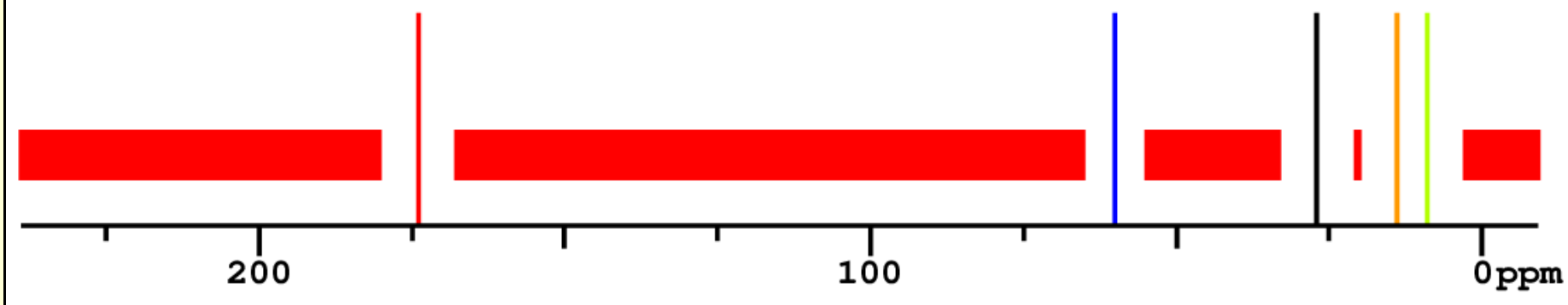
Structure	Similarity Measure
	<p>Deviation = 7.25 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_8O</math></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">RJYJUVQCQXAQWHG</a></p>
Predicted Chemical Shiftvalues	Matching Map





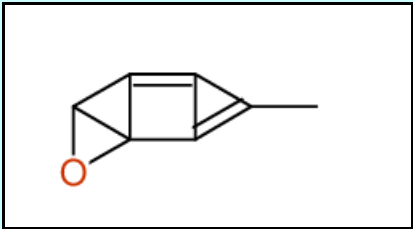
Experimental shift values

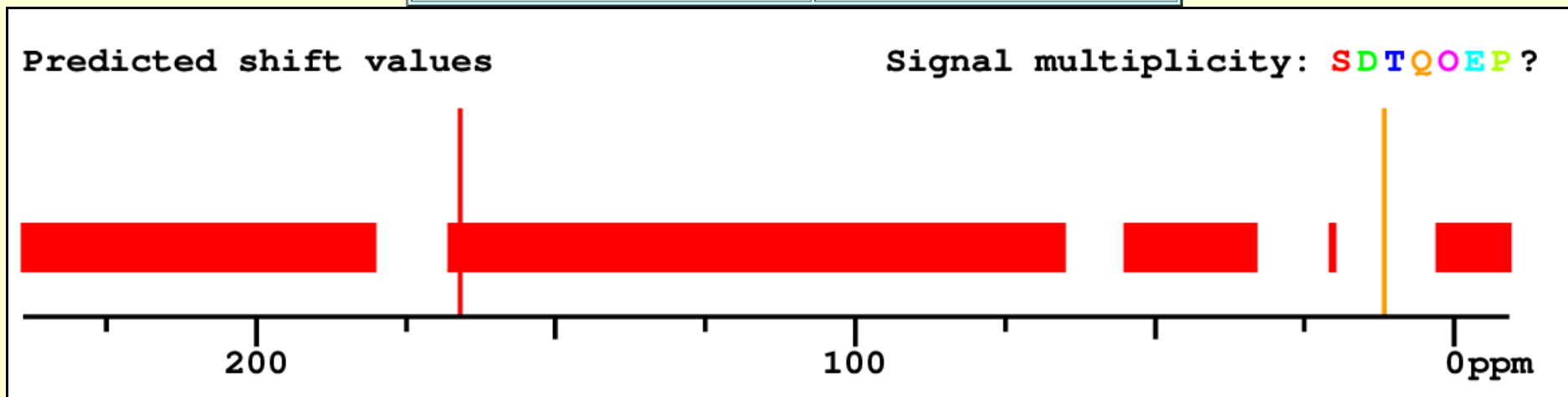
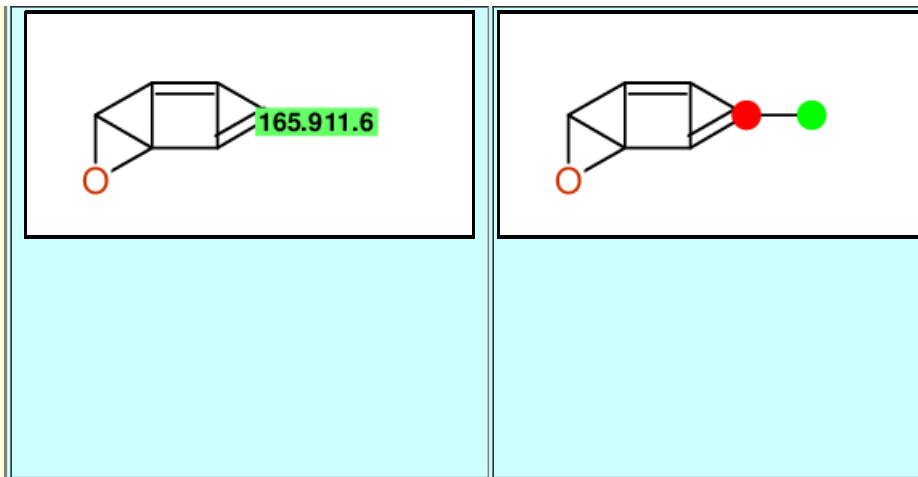
No line in reference: 



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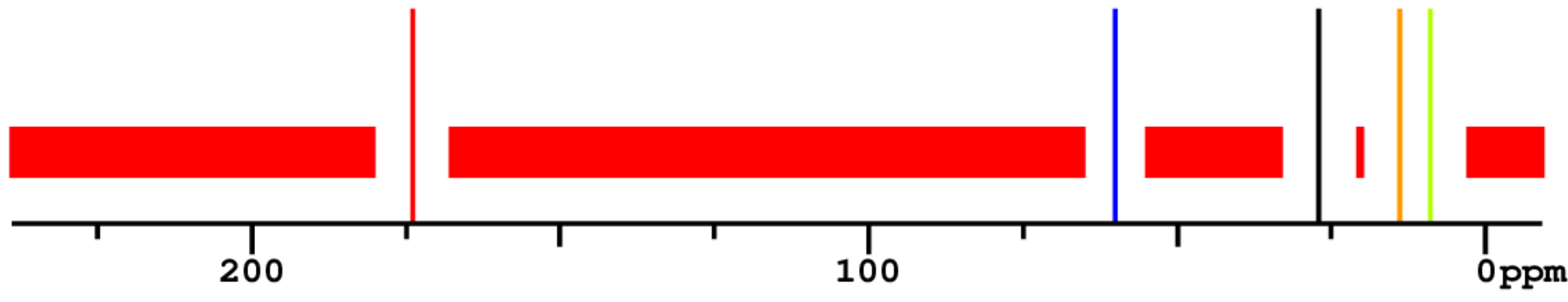
### Structure Proposal #26

Structure	Similarity Measure
	<p>Deviation = 7.49 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_7H_4O</math></p> <p>MWT = 104.08</p> <p>Search Web for this structure: <a href="#">XYCXRSMOQENPEQ</a></p>
Predicted Chemical Shiftvalues	Matching Map



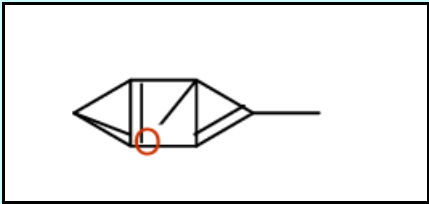
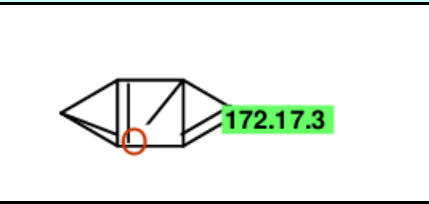
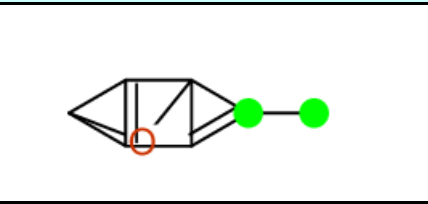
Experimental shift values

No line in reference: 



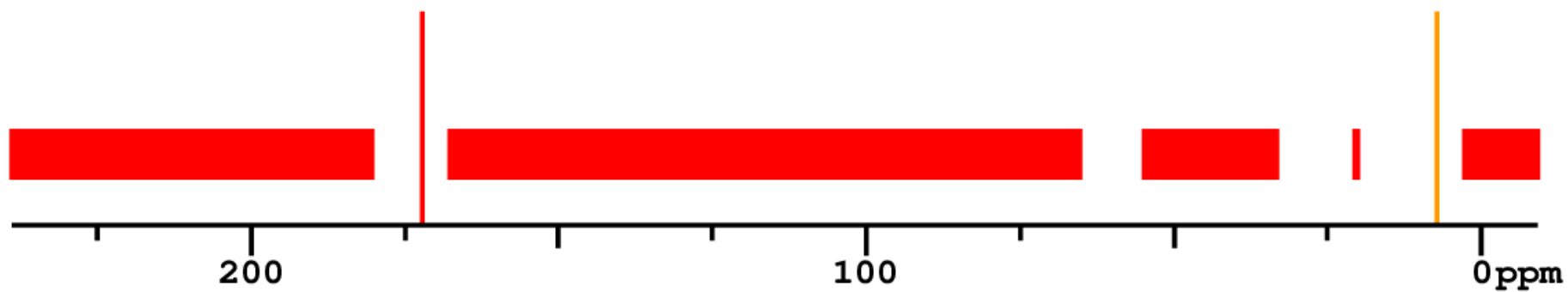
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### Structure Proposal #27

Structure	Similarity Measure
	Deviation = 7.82 ppm Similarity = 100 %  C <sub>7</sub> H <sub>4</sub> O  MWT = 104.08 Search Web for this structure: <a href="#">YXVQMKXJOHSUEX</a>
Predicted Chemical Shiftvalues	Matching Map
	

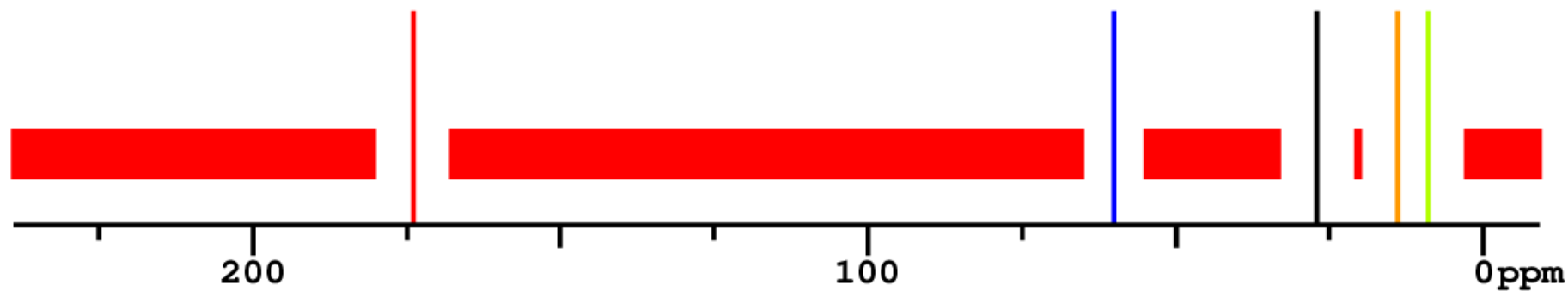
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

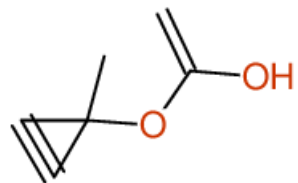
No line in reference: [red bar]



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### Structure Proposal #28

Structure	Similarity Measure



Deviation = 8.16 ppm  
Similarity = 100 %

$C_6H_{10}O_2$

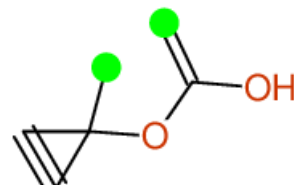
MWT = 110.07

Search Web for this structure:

[QYPIIJZABARONQ](#)

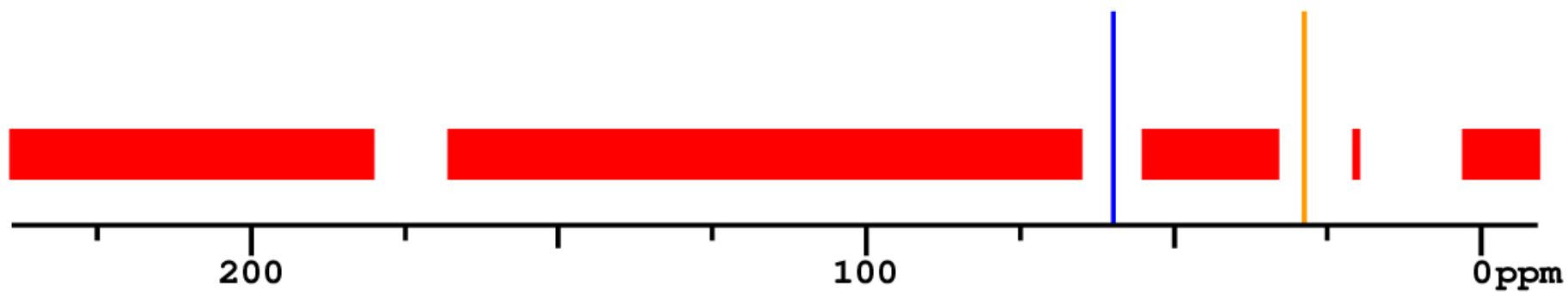
Predicted Chemical  
Shiftvalues

Matching Map



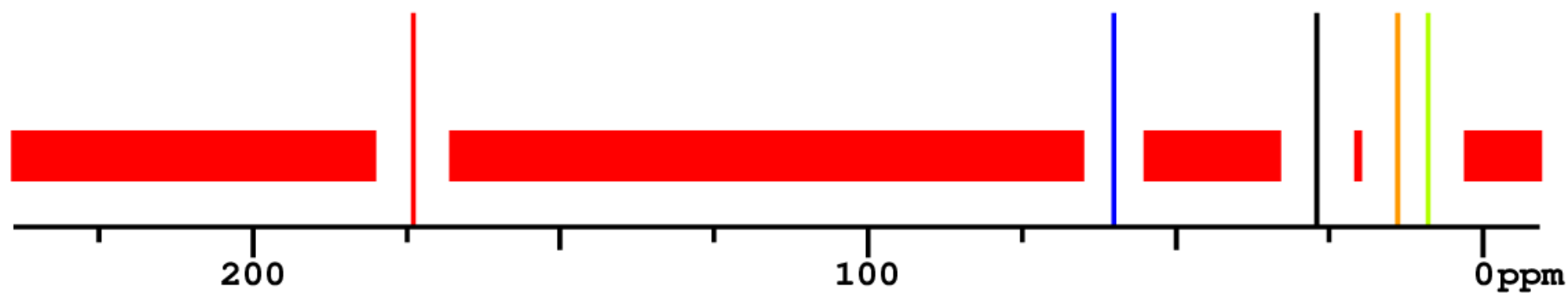
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

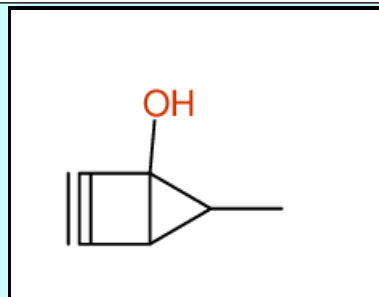
No line in reference: [red bar]



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### Structure Proposal #29

Structure	Similarity Measure



Deviation = 8.28 ppm  
 Similarity = 50 %  
 (Different pattern)



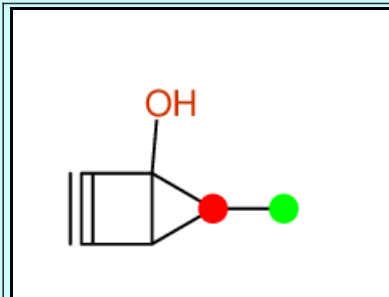
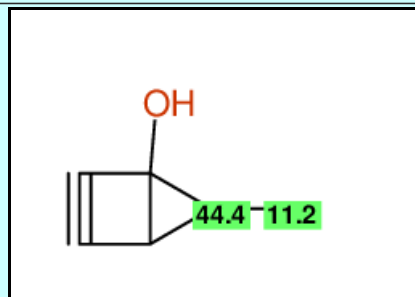
MWT = 94.07

Search Web for this structure:

[GJAGHYKQEPSNN](#)

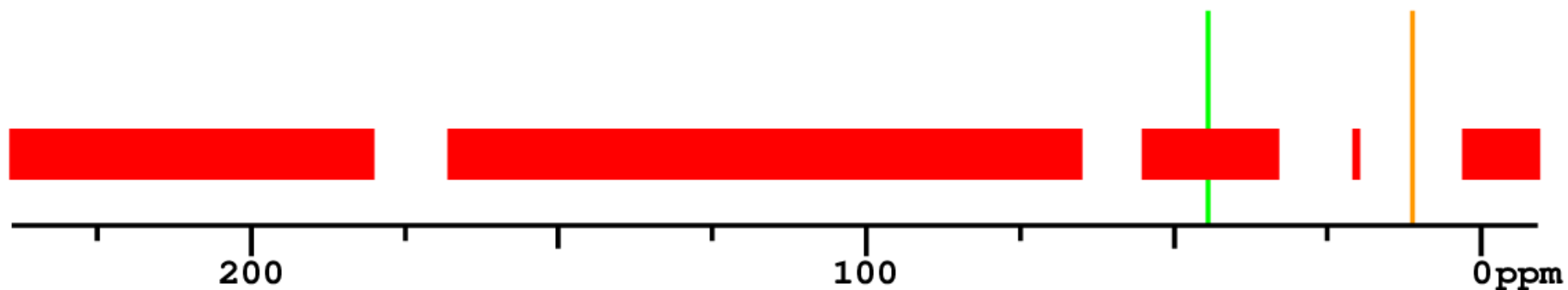
Predicted Chemical Shiftvalues

Matching Map



Predicted shift values

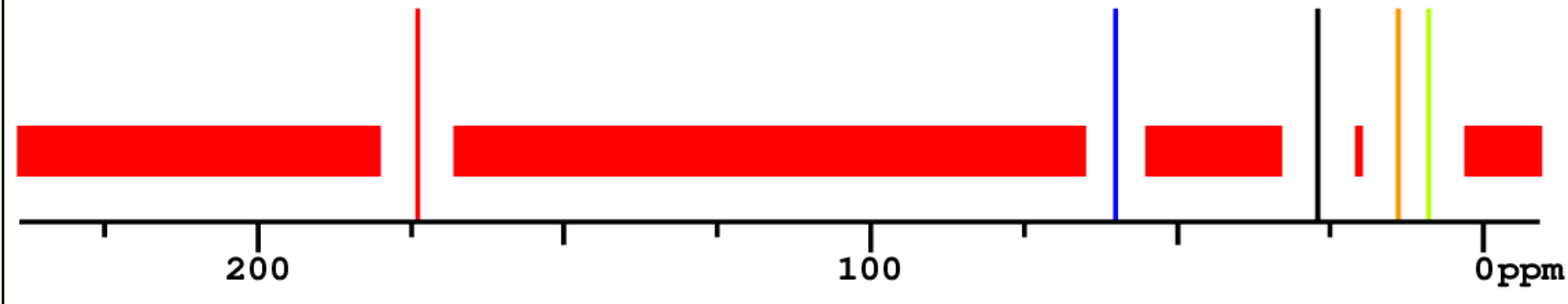
Signal multiplicity: **S****D****T****Q****O****E****P**?





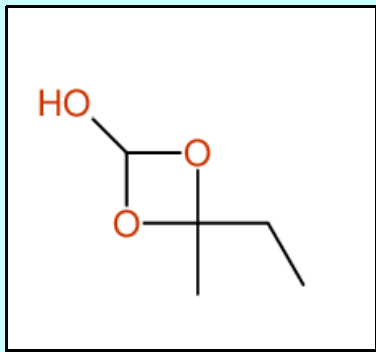
Experimental shift values

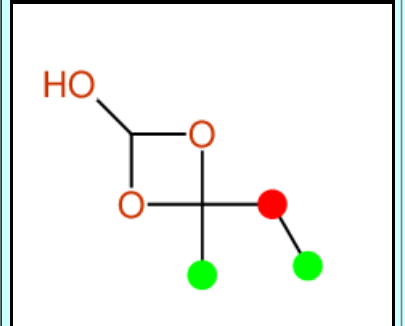
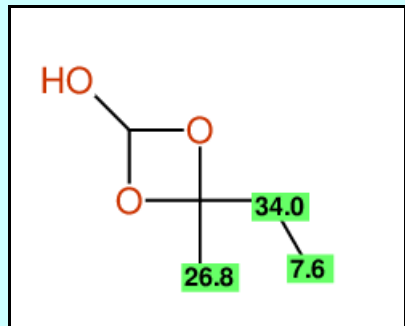
No line in reference: 



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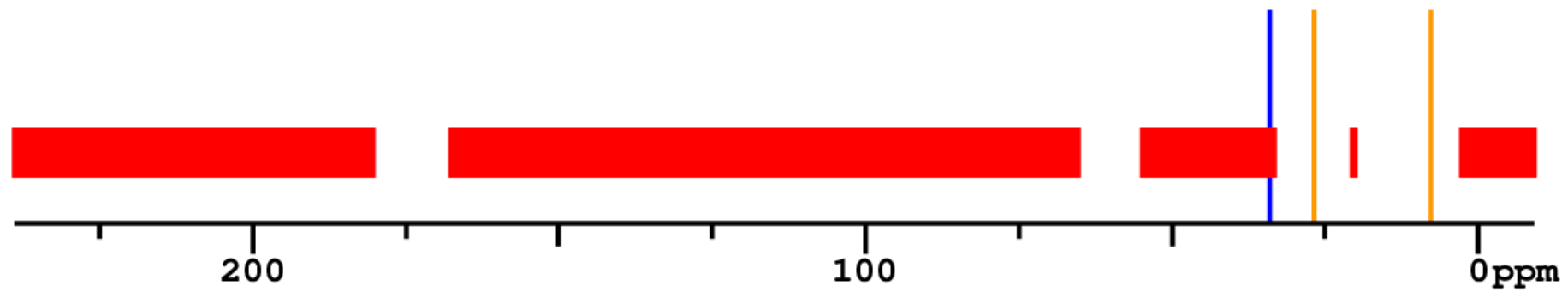
### Structure Proposal #30

Structure	Similarity Measure
	<p>Deviation = 8.34 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_5H_{10}O_3</math></p> <p>MWT = 118.06</p> <p>Search Web for this structure: <a href="#">CMMVOYHDZZWQKE</a></p>
Predicted Chemical Shiftvalues	Matching Map



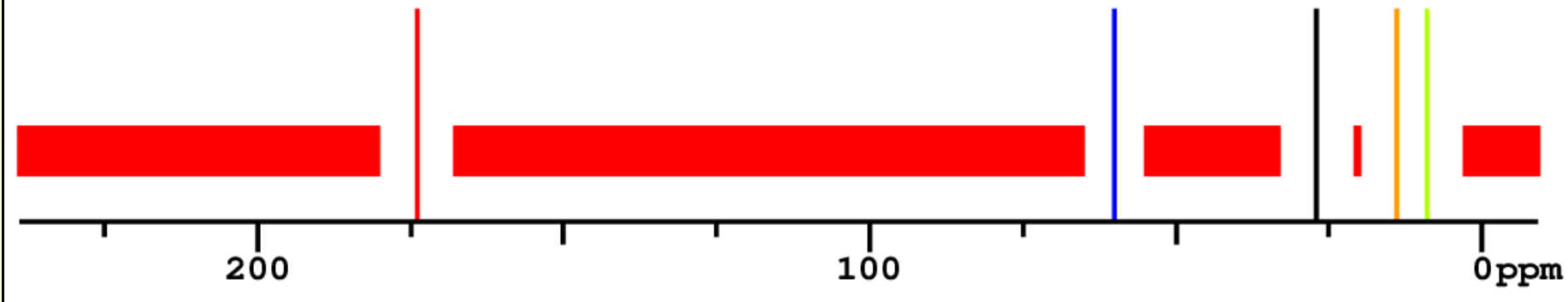
Predicted shift values

Signal multiplicity: S D T Q O E P ?



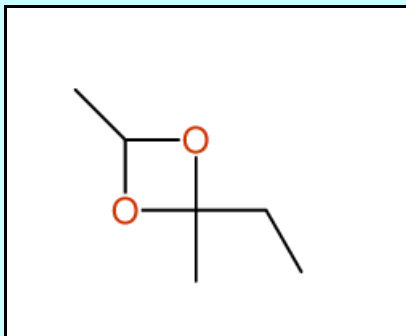
Experimental shift values

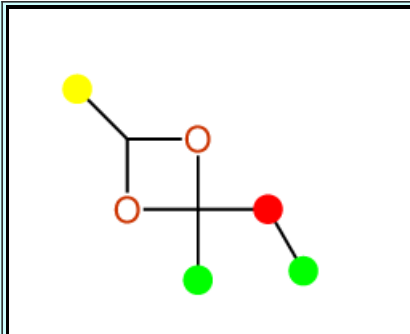
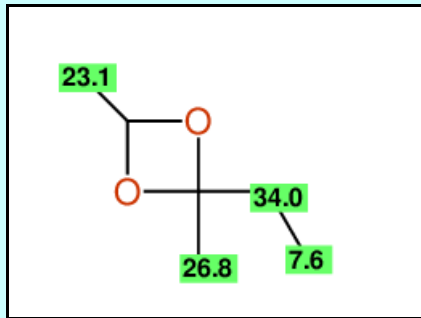
No line in reference: 



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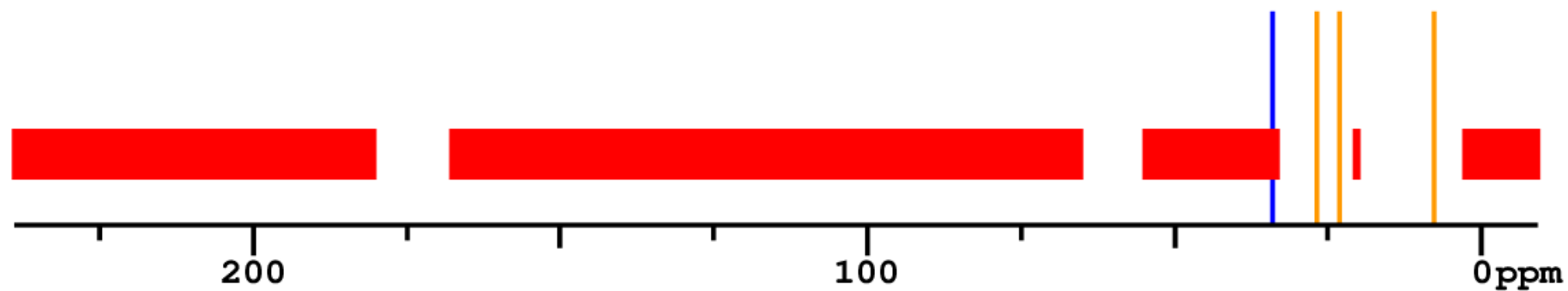
### Structure Proposal #31

Structure	Similarity Measure
	<p>Deviation = 8.49 ppm Similarity = 63 % (Different pattern)</p> <p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.07</p> <p>Search Web for this structure: <a href="#">HRHKYDWQVMBLPA</a></p>
Predicted Chemical Shiftvalues	Matching Map



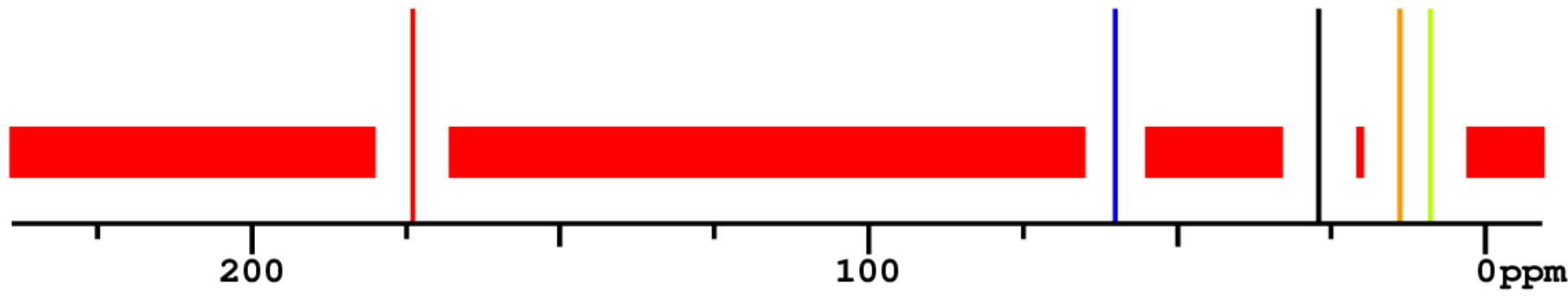
Predicted shift values

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



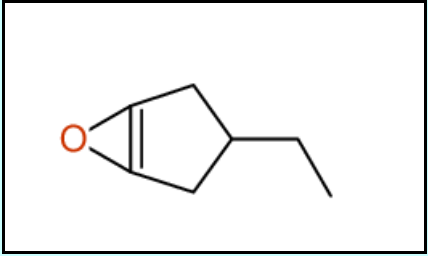
Experimental shift values

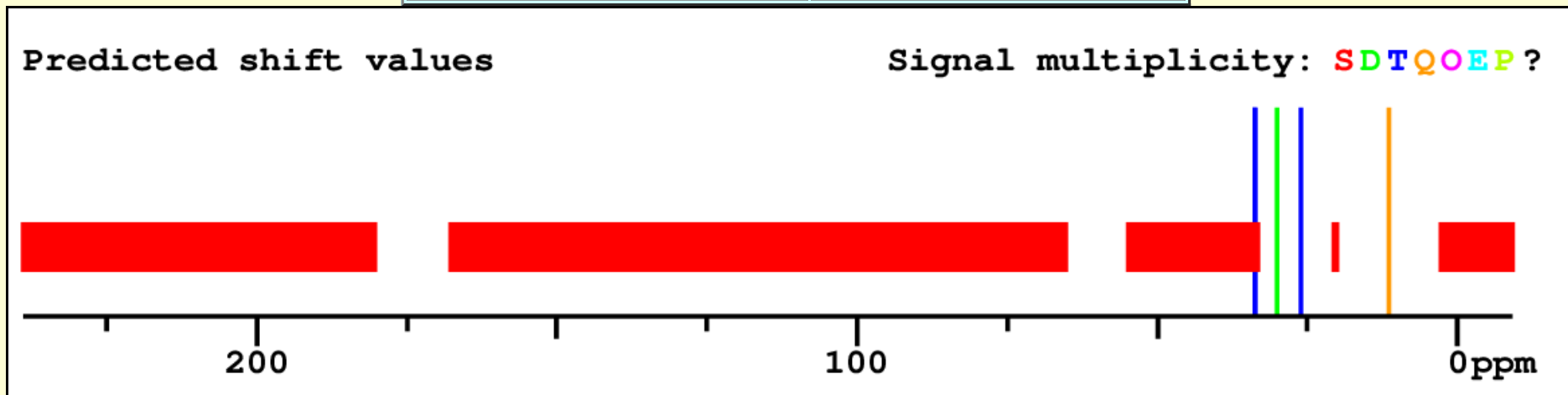
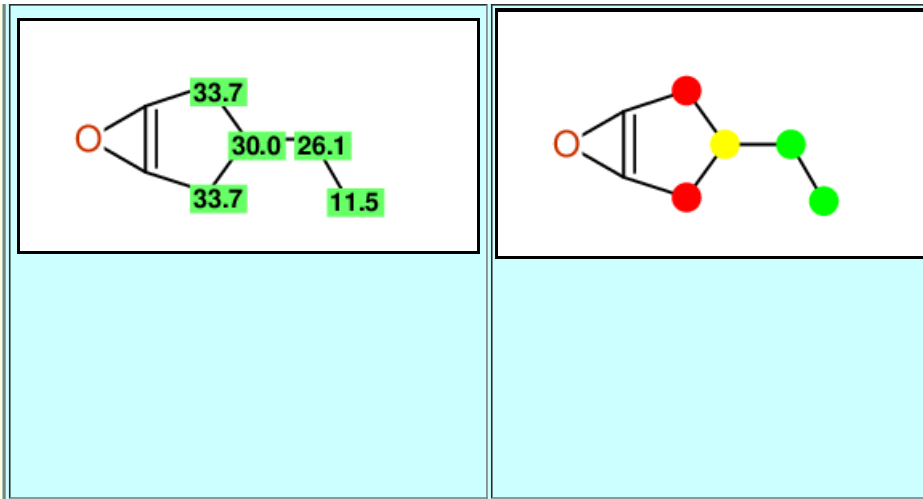
No line in reference: 



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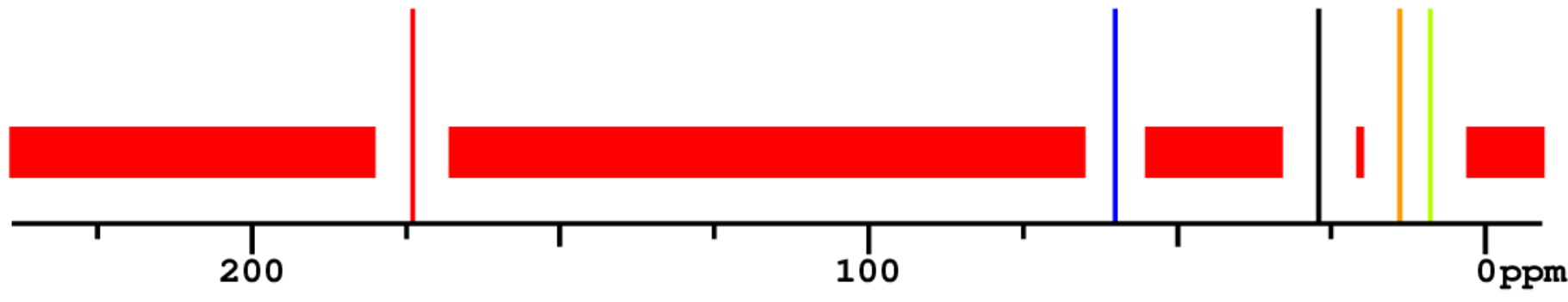
Structure Proposal #32

Structure	Similarity Measure
 <p>The chemical structure shows a bicyclic system consisting of a five-membered ring fused to a four-membered ring. An oxygen atom is part of the five-membered ring. An ethyl group is attached to the four-membered ring.</p>	<p>Deviation = 8.74 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_7H_{10}O</math></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">SIEWESXVNIJEJB</a></p>
Predicted Chemical Shiftvalues	Matching Map



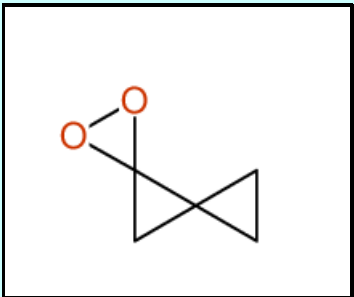
Experimental shift values

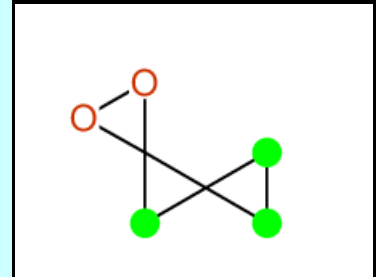
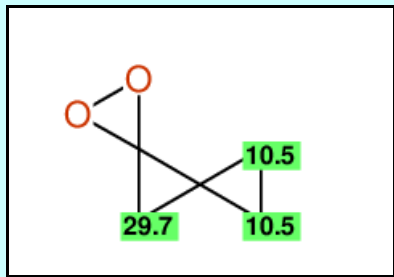
No line in reference: 



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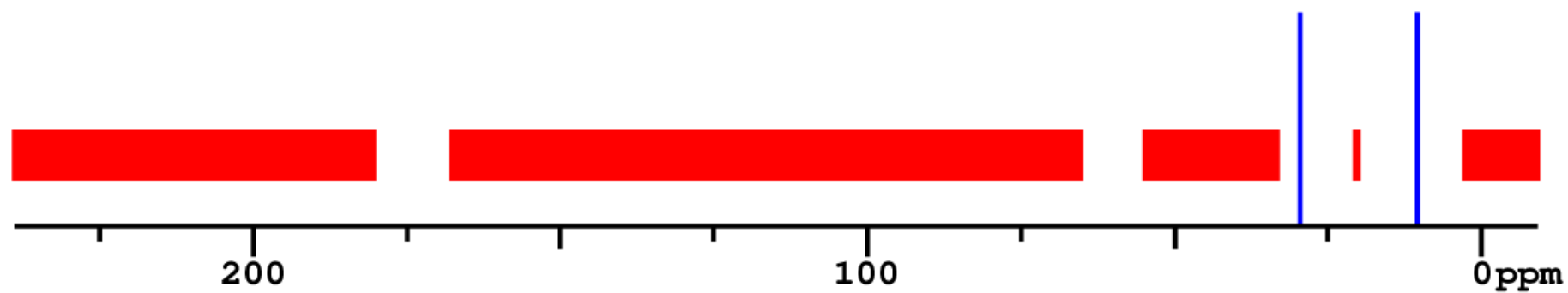
### Structure Proposal #33

Structure	Similarity Measure
	Deviation = 8.75 ppm Similarity = 100 %  $C_5H_6O_2$  MWT = 98.06  Search Web for this structure: <a href="#">WGAVRTDGCNTZGM</a>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

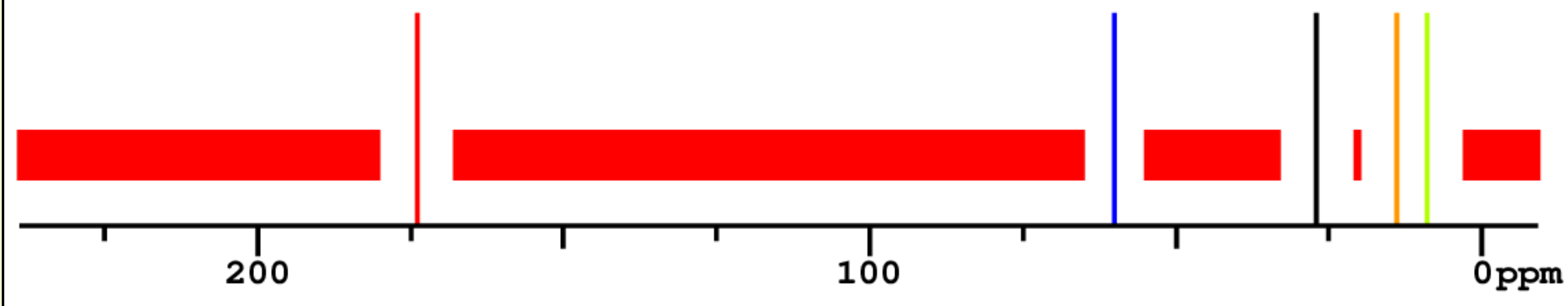
Signal multiplicity: S D T Q O E P ?





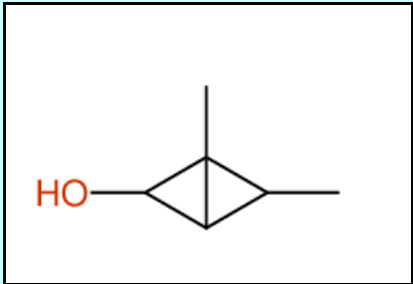
Experimental shift values

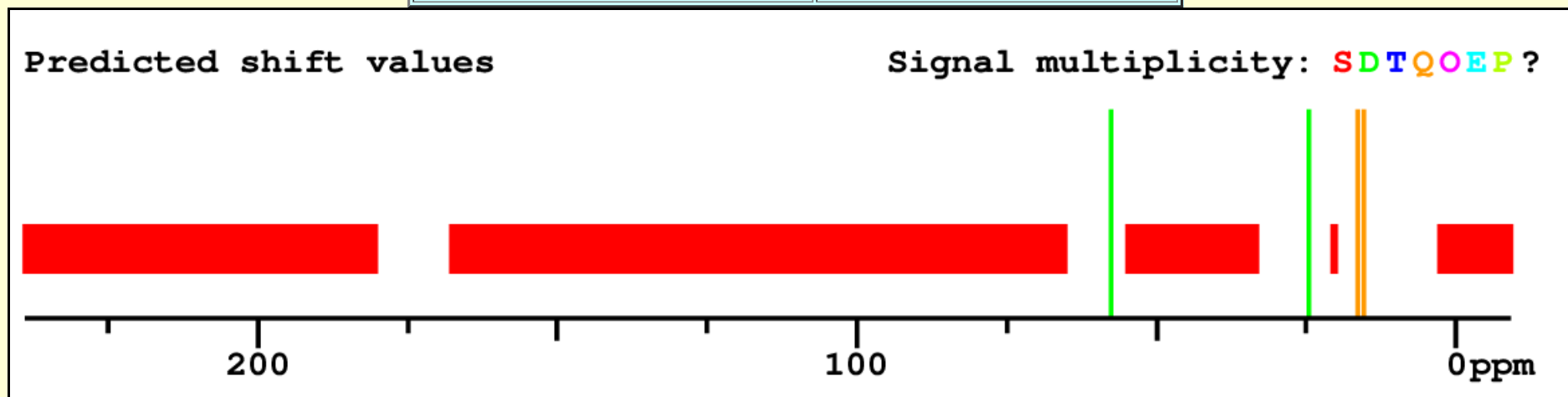
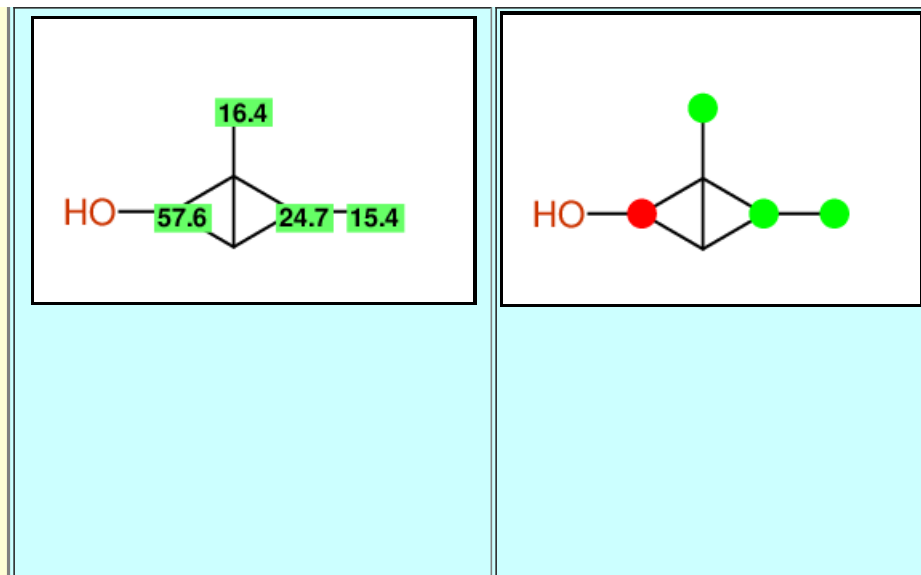
No line in reference: 



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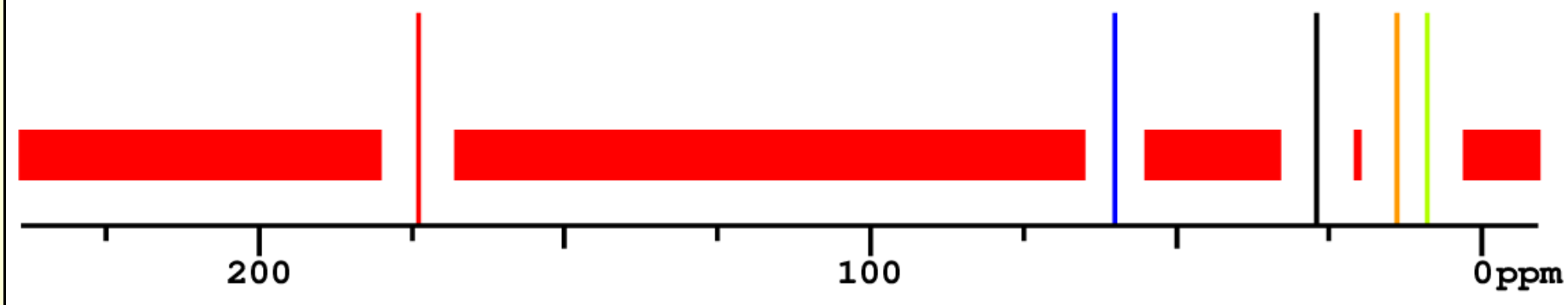
### Structure Proposal #34

Structure	Similarity Measure
 <p>Chemical structure of 2-methylcyclohexanol, showing a cyclohexane ring with a hydroxyl group (HO) and a methyl group (CH<sub>3</sub>) attached to the same carbon atom.</p>	<p>Deviation = 8.75 ppm Similarity = 75 %</p> <p><chem>C6H10O</chem></p> <p>MWT = 98.07</p> <p>Search Web for this structure: <a href="#">NEQPKAVUXMQCHO</a></p>
Predicted Chemical Shiftvalues	Matching Map



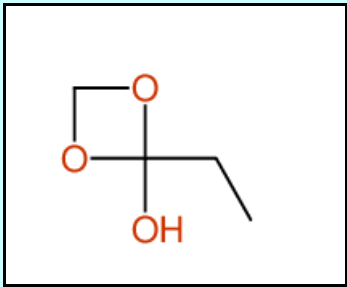
Experimental shift values

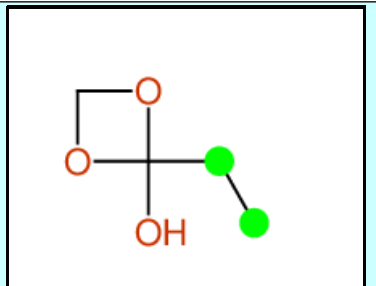
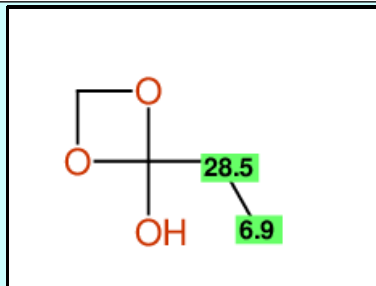
No line in reference: 



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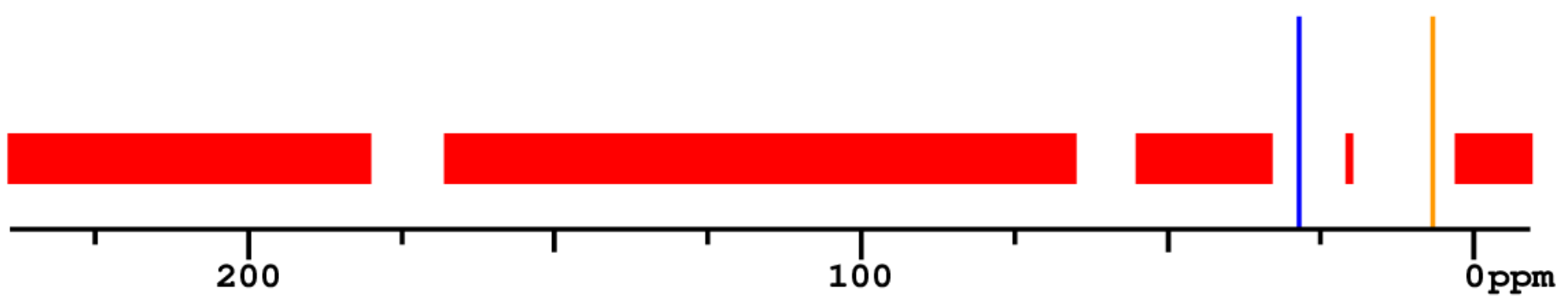
### Structure Proposal #35

Structure	Similarity Measure
	Deviation = 8.90 ppm Similarity = 100 %  $C_4H_8O_3$  MWT = 104.04  Search Web for this structure:  <a href="#">CIDICLGXRQBWEQ</a>
Predicted Chemical Shiftvalues	Matching Map



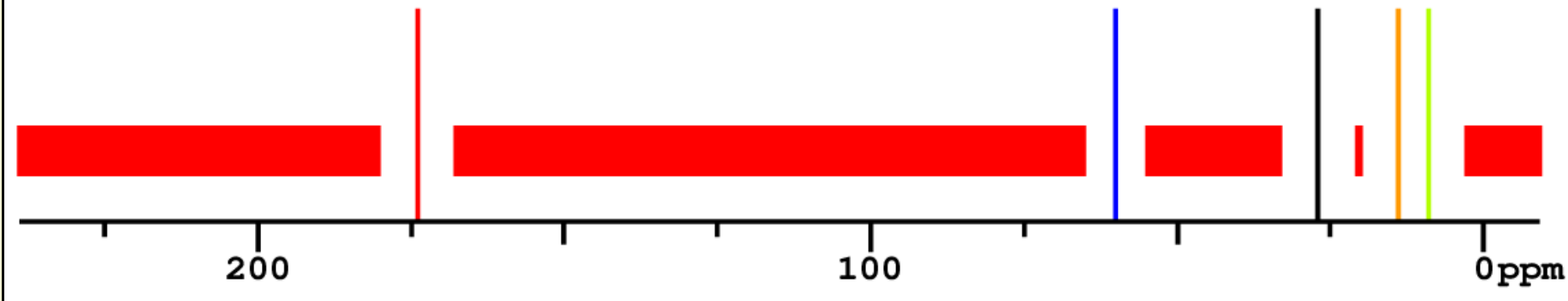
Predicted shift values

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



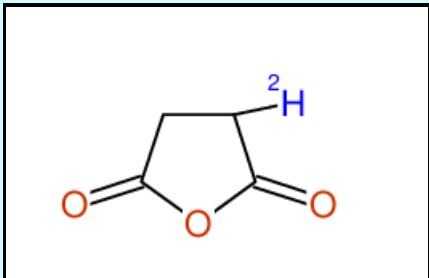
Experimental shift values

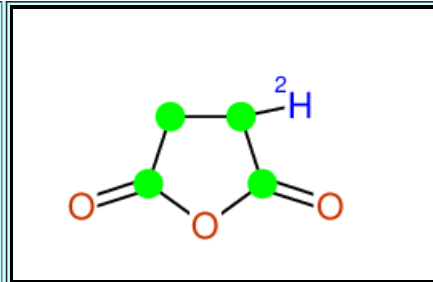
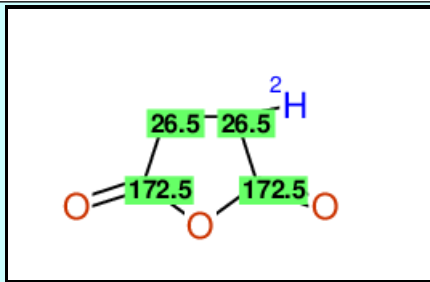
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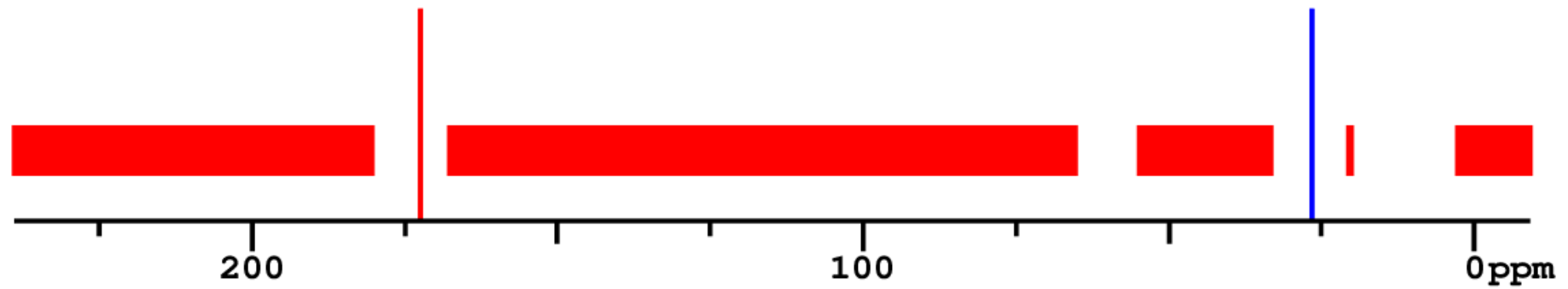
### Structure Proposal #36

Structure	Similarity Measure
	Deviation = 9.10 ppm Similarity = 100 %  $C_4H_4O_3$  MWT = 101.04 Search Web for this structure: <a href="#">RINCXYOBBGOEEQ</a> <a href="#">Availability</a>
Predicted Chemical Shiftvalues	Matching Map



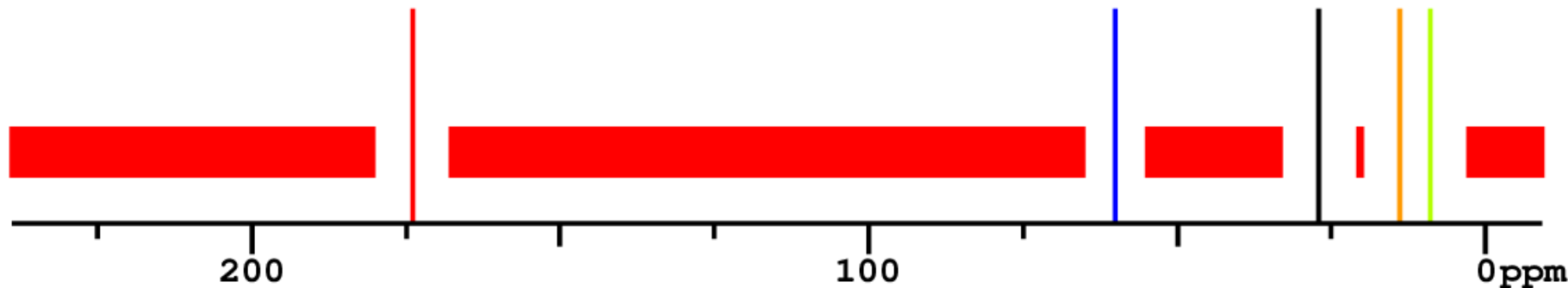
Predicted shift values

Signal multiplicity: S D T Q O E P ?



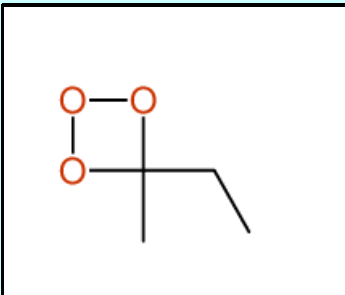
Experimental shift values

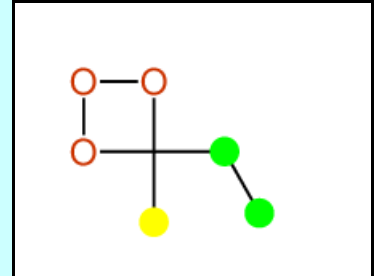
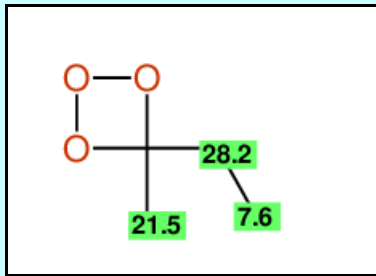
No line in reference: 



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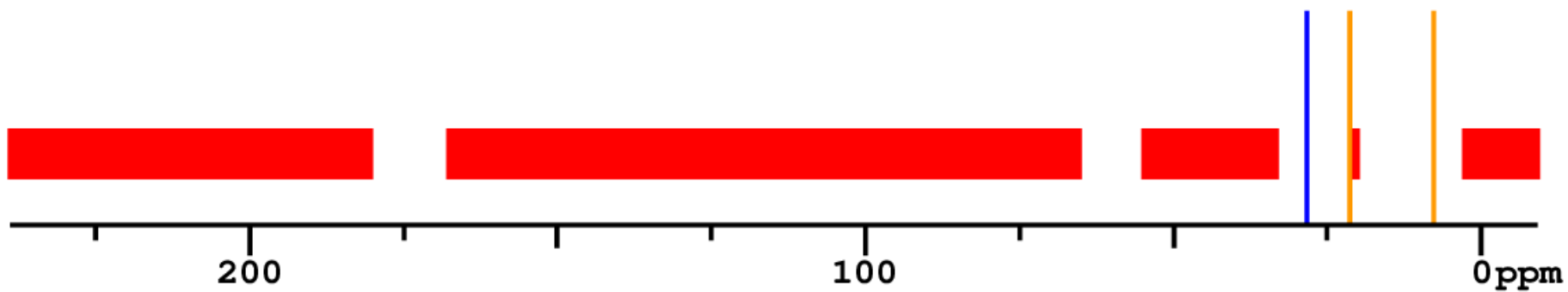
### Structure Proposal #37

Structure	Similarity Measure
	<p>Deviation = 9.11 ppm Similarity = 83 %</p> <p><math>C_4H_8O_3</math></p> <p>MWT = 104.04</p> <p>Search Web for this structure: <a href="#">CZUKTAOQHAZAPX</a></p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

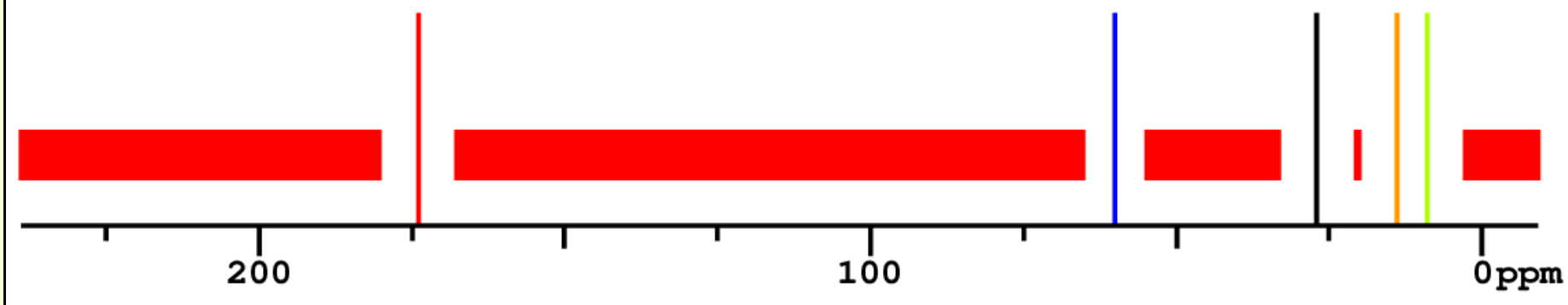
Signal multiplicity: S D T Q O E P ?





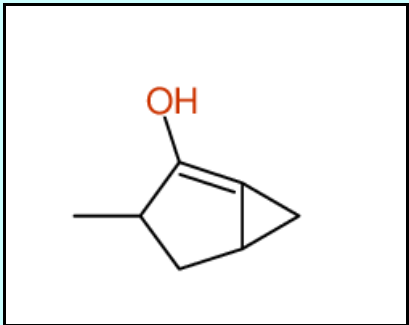
Experimental shift values

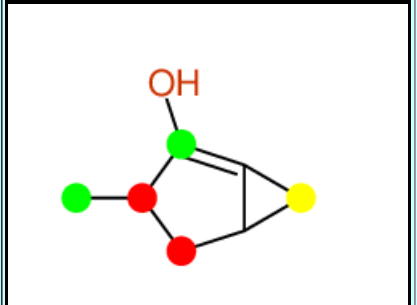
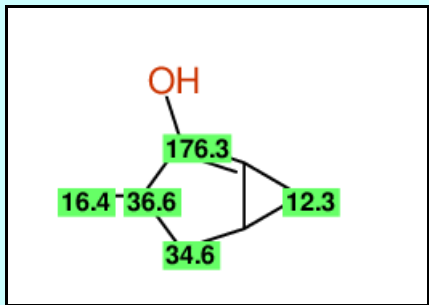
No line in reference: 



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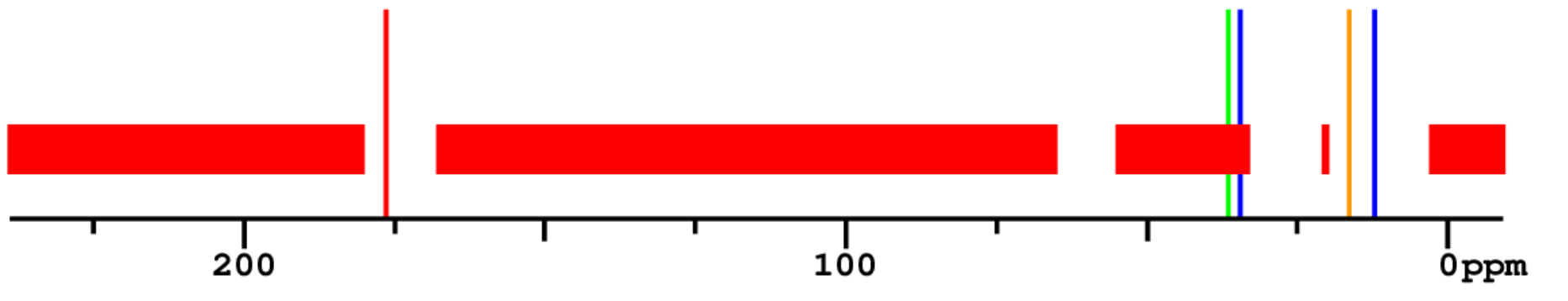
### Structure Proposal #38

Structure	Similarity Measure
	<p>Deviation = 9.12 ppm Similarity = 50 % (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



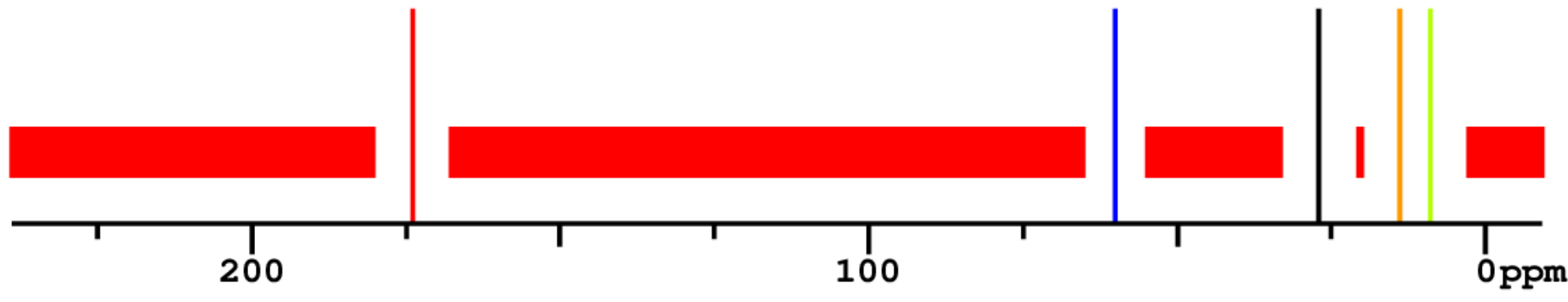
Predicted shift values

Signal multiplicity: S D T Q O E P ?



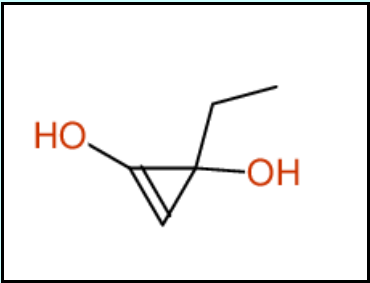
Experimental shift values

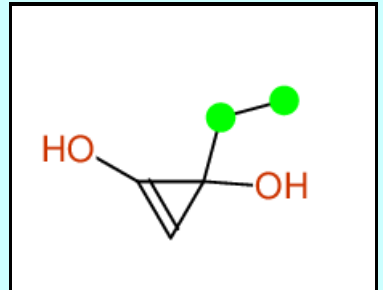
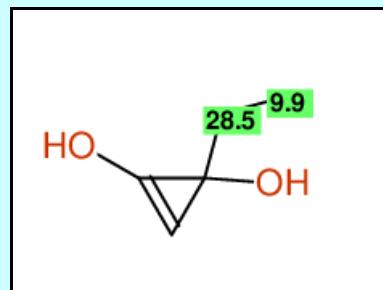
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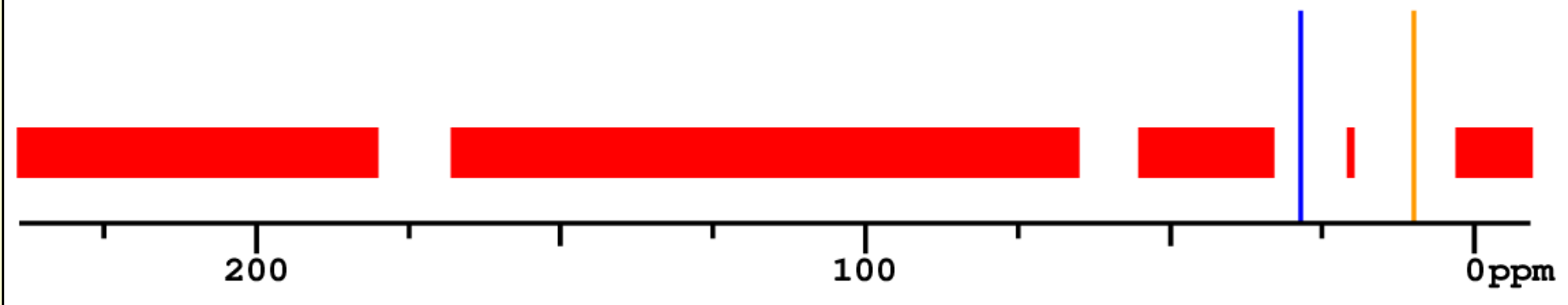
Structure Proposal #39

Structure	Similarity Measure
	Deviation = 9.17 ppm Similarity = 100 %  C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>  MWT = 100.06  Search Web for this structure:  <a href="#">LYEDKJATIQMCTQ</a>
Predicted Chemical Shiftvalues	Matching Map



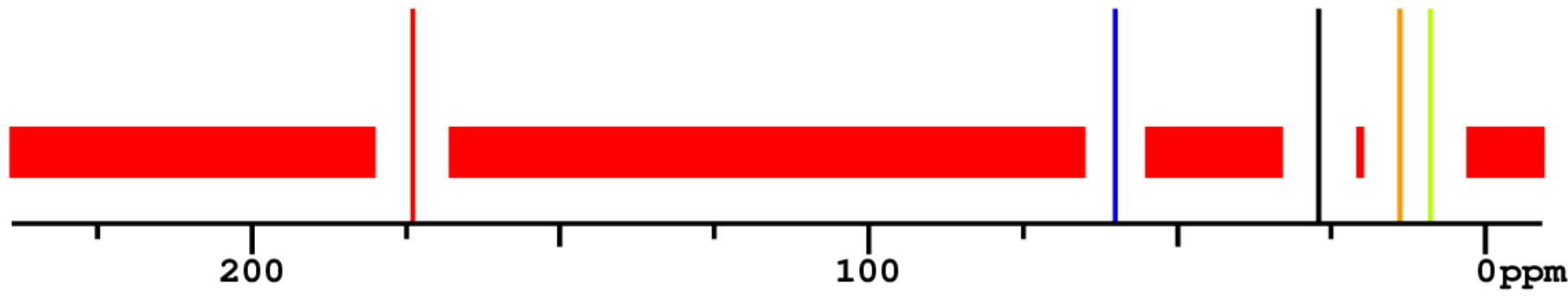
Predicted shift values

Signal multiplicity: S D T Q O E P ?



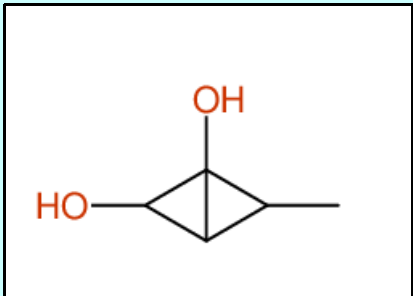
Experimental shift values

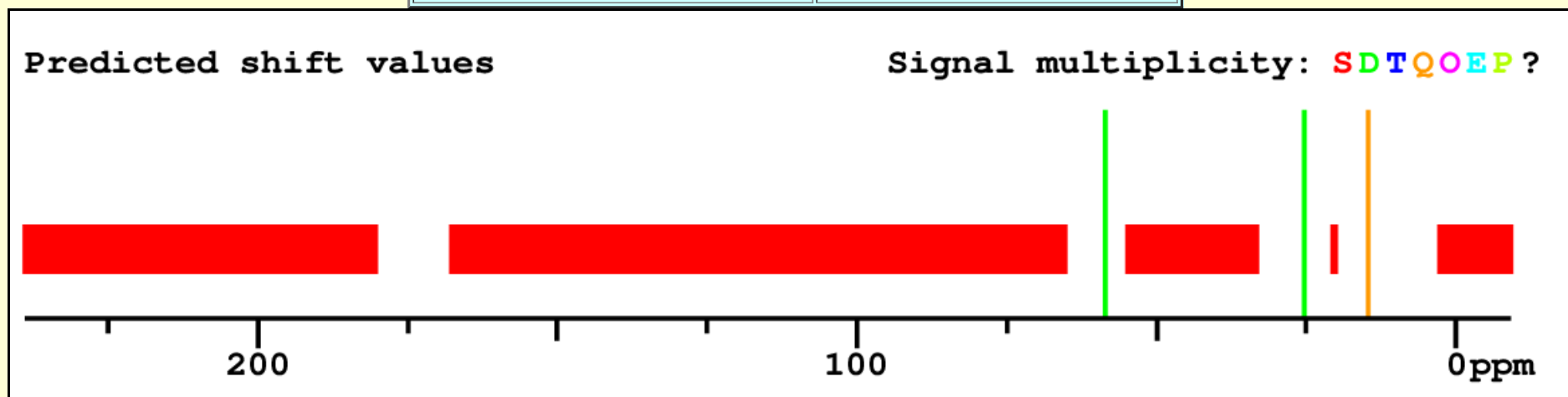
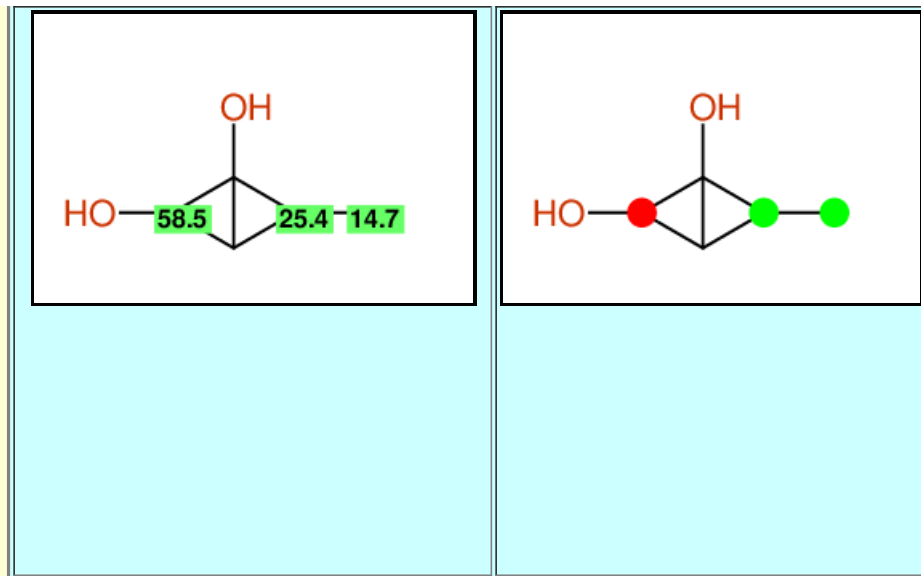
No line in reference: 



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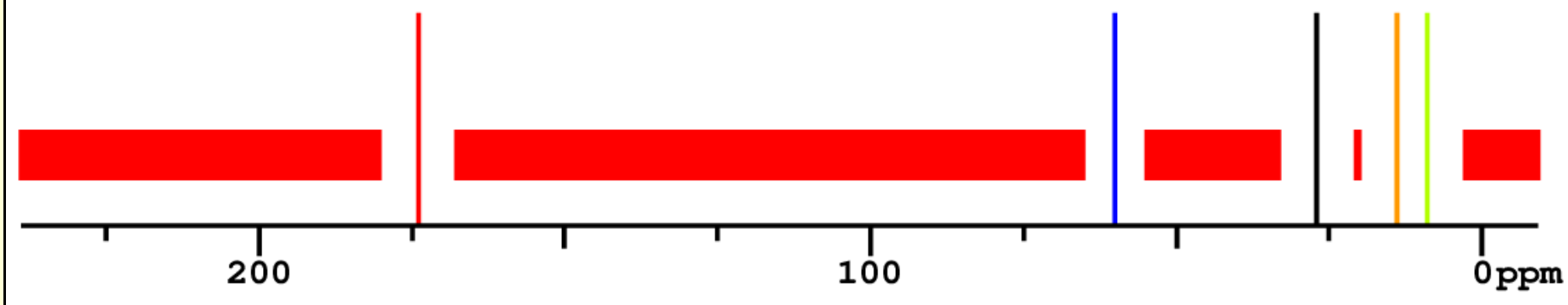
### Structure Proposal #40

Structure	Similarity Measure
 <p>The chemical structure shown is menthol, a bicyclic monoterpene alcohol. It consists of a decalin ring system with a hydroxyl group (-OH) at the 1-position and an isopropyl group at the 2-position.</p>	<p>Deviation = 9.31 ppm Similarity = 67 %</p> <p><math>C_5H_8O_2</math></p> <p>MWT = 100.06</p> <p>Search Web for this structure: <a href="#">XLPULUZDEMTOLL</a></p>
Predicted Chemical Shiftvalues	Matching Map



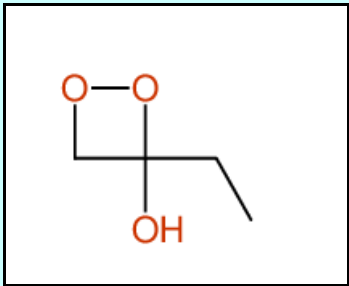
Experimental shift values

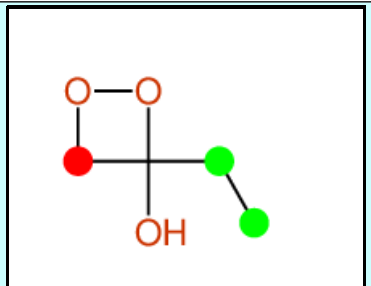
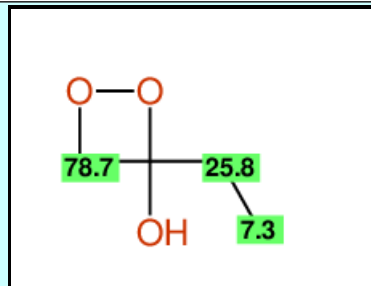
No line in reference: 



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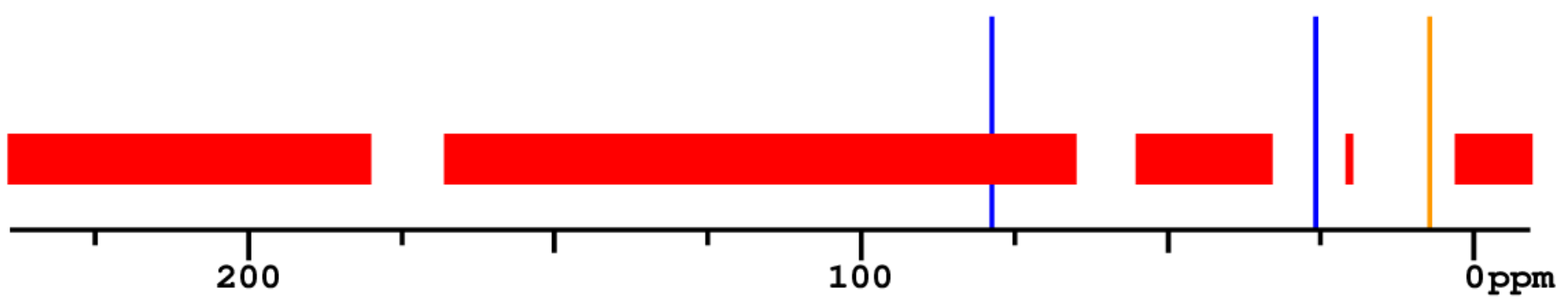
### Structure Proposal #41

Structure	Similarity Measure
	<p>Deviation = 9.40 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_4H_8O_3</math></p> <p>MWT = 104.04</p> <p>Search Web for this structure: <a href="#">LPMMUOPZFPDUGT</a></p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

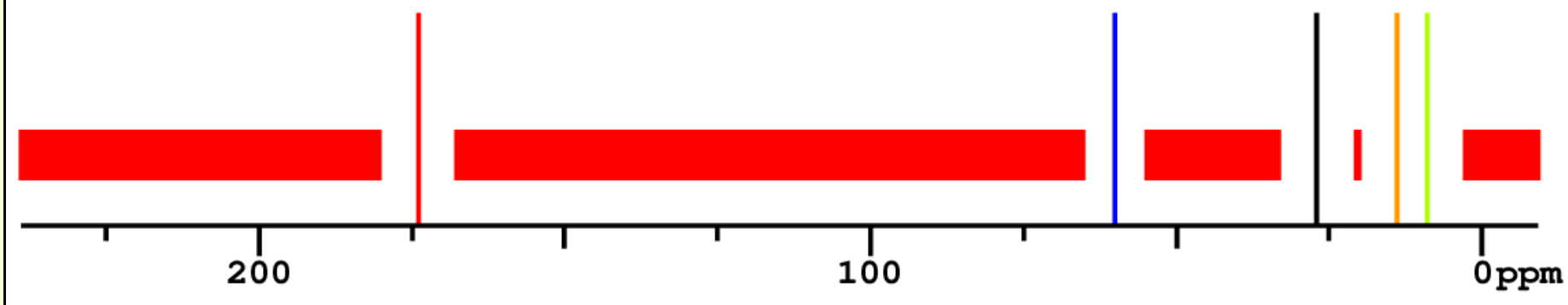
Signal multiplicity: S D T Q O E P ?





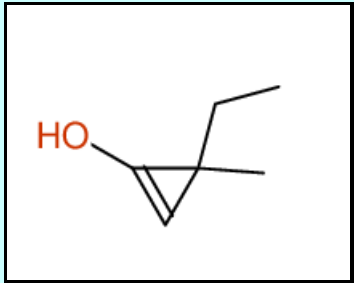
Experimental shift values

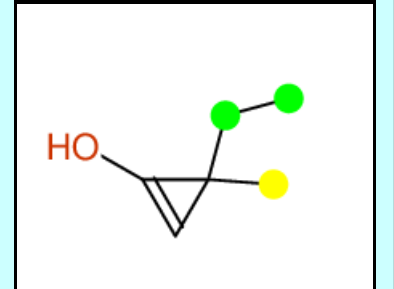
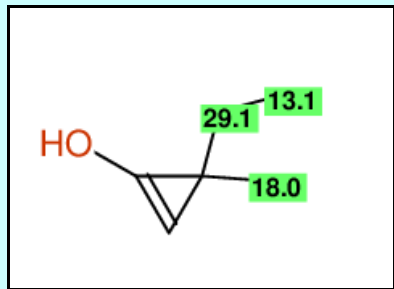
No line in reference: 



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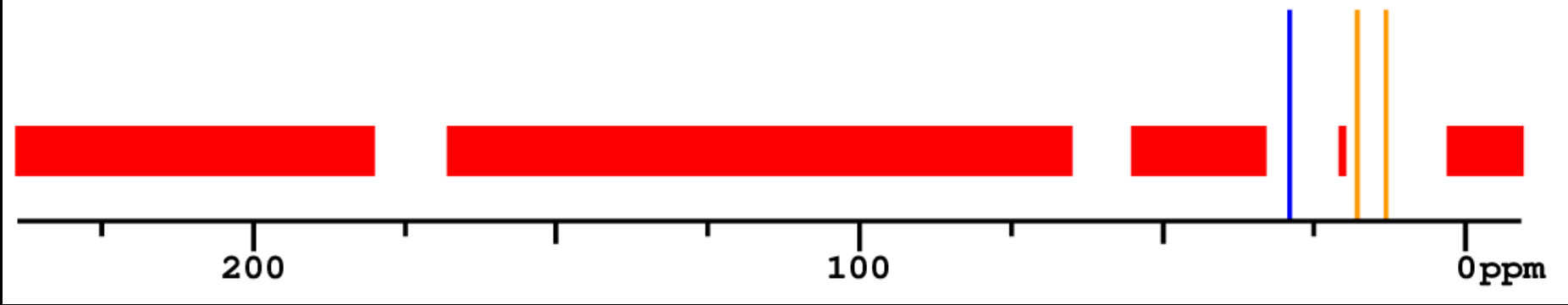
### Structure Proposal #42

Structure	Similarity Measure
	Deviation = 9.40 ppm Similarity = 83 %  $C_6H_{10}O$  MWT = 98.07  Search Web for this structure:  <a href="#">NTSMDEJACBLTSE</a>
Predicted Chemical Shiftvalues	Matching Map



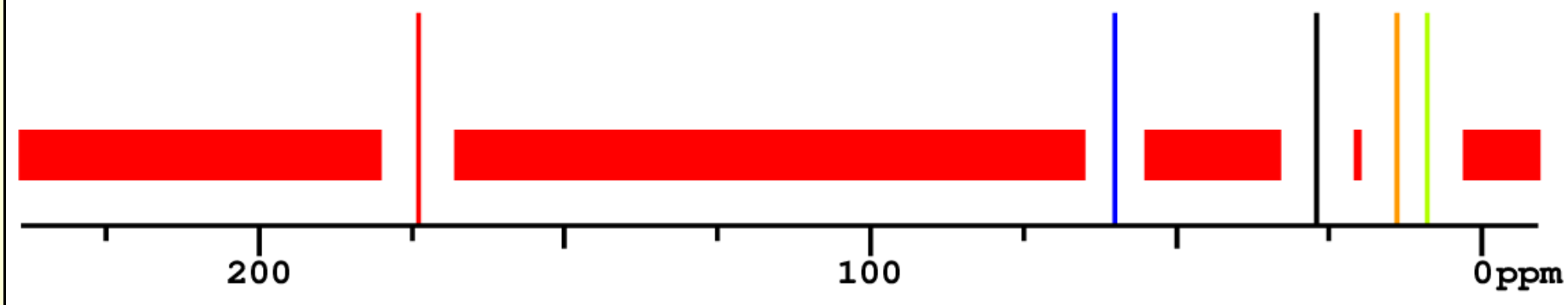
Predicted shift values

Signal multiplicity: S D T Q O E P ?



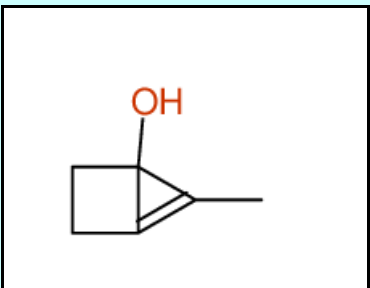
Experimental shift values

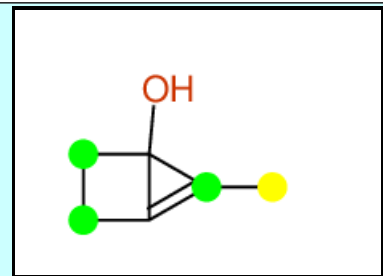
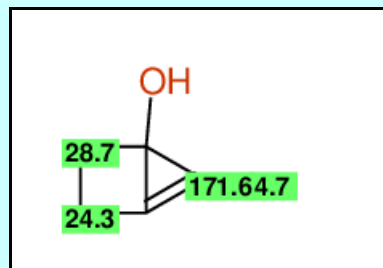
No line in reference: 



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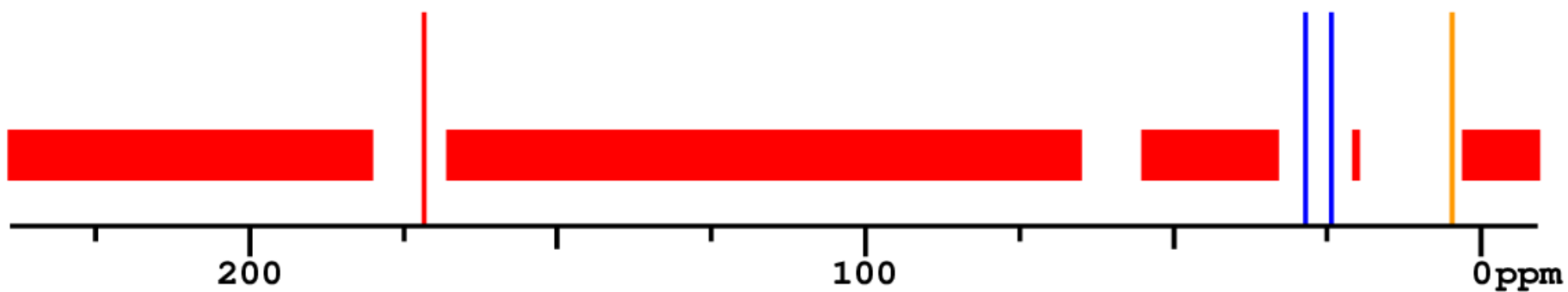
### Structure Proposal #43

Structure	Similarity Measure
	Deviation = 9.51 ppm Similarity = 88 %  C <sub>6</sub> H <sub>8</sub> O  MWT = 96.07  Search Web for this structure: <a href="#">WPNREIWMCOZWLX</a>
Predicted Chemical Shiftvalues	Matching Map



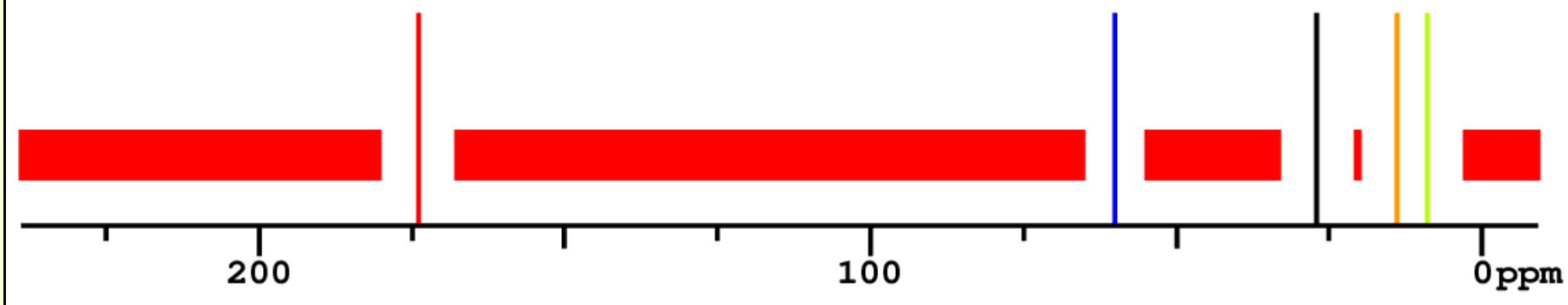
Predicted shift values

Signal multiplicity: S D T Q O E P ?



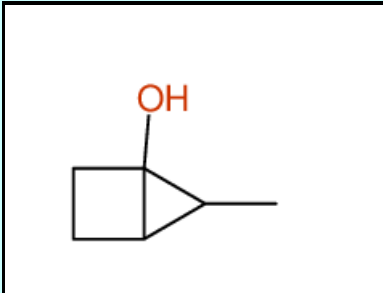
Experimental shift values

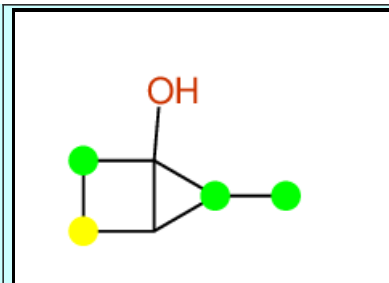
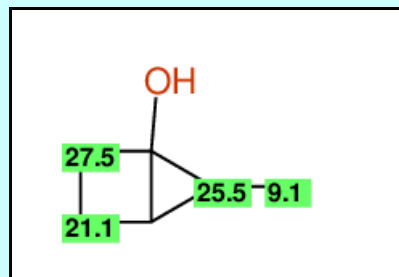
No line in reference: 



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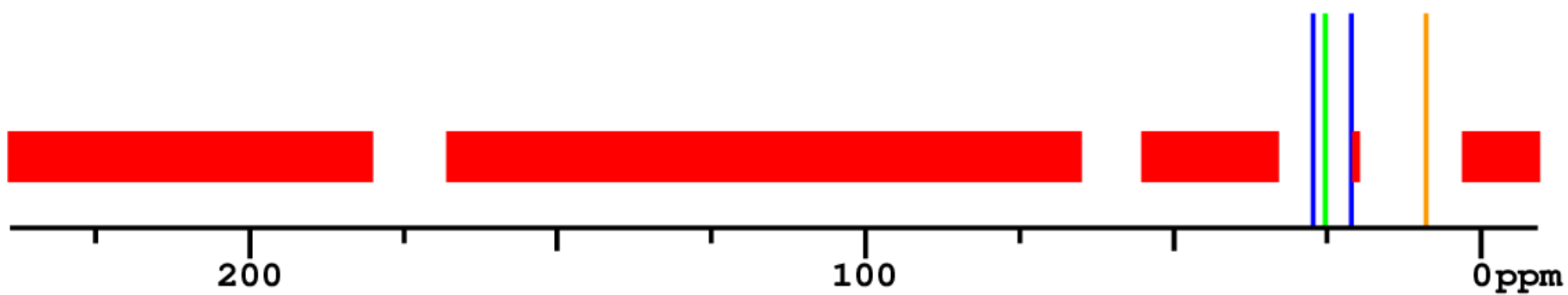
#### Structure Proposal #44

Structure	Similarity Measure
	Deviation = 9.58 ppm Similarity = 88 %  $C_6H_{10}O$  MWT = 98.07  Search Web for this structure:  <a href="#">JXAXUFPFGOOMCOO</a>
Predicted Chemical Shiftvalues	Matching Map



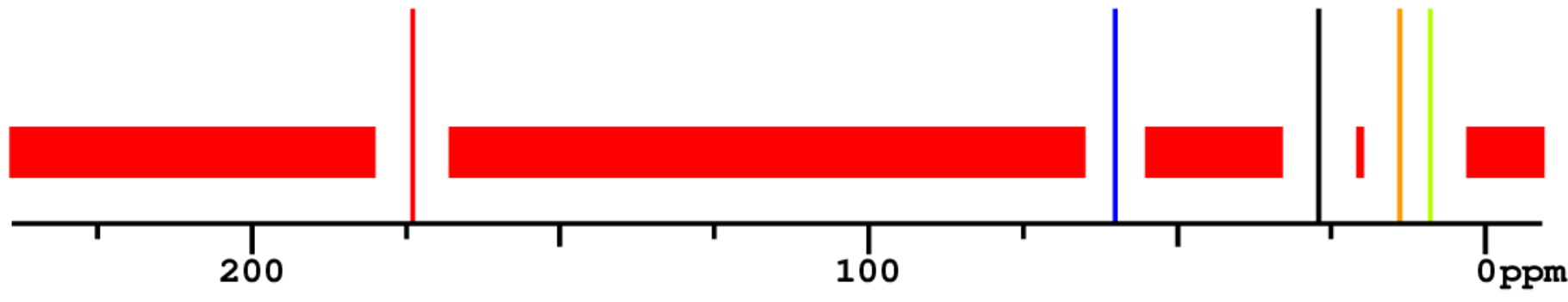
Predicted shift values

Signal multiplicity: S D T Q O E P ?



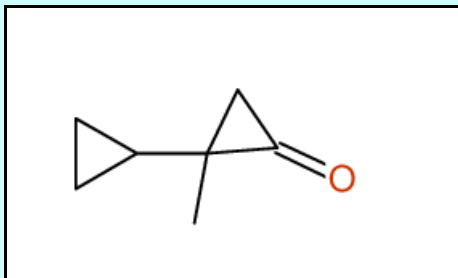
Experimental shift values

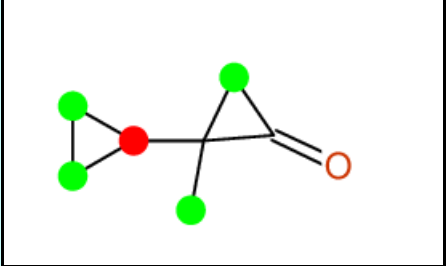
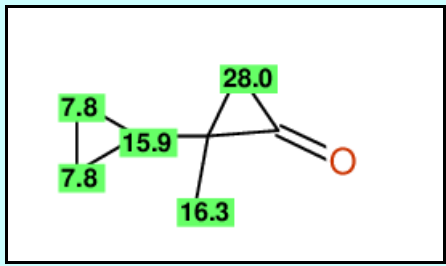
No line in reference: 



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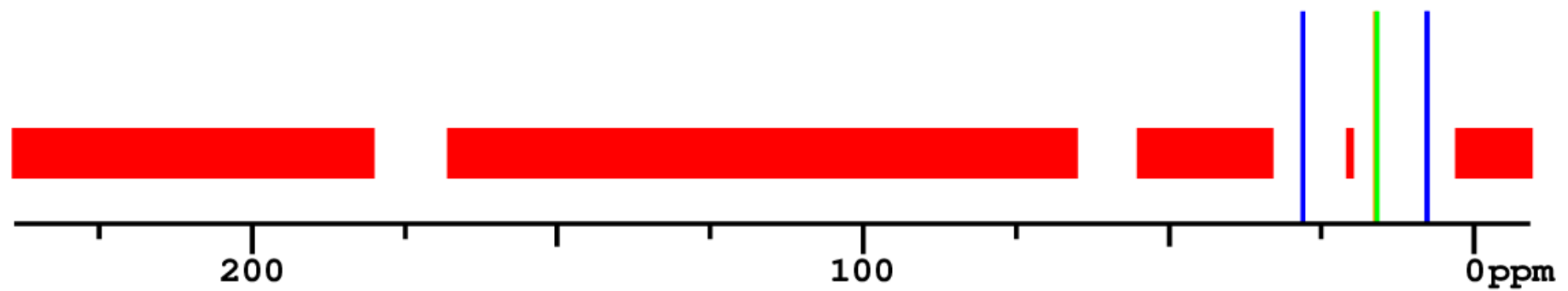
### Structure Proposal #45

Structure	Similarity Measure
	Deviation = 9.63 ppm Similarity = 80 %  C <sub>7</sub> H <sub>10</sub> O  MWT = 110.08 Search Web for this structure: <a href="#">IXMZEVVZABSMMG</a>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

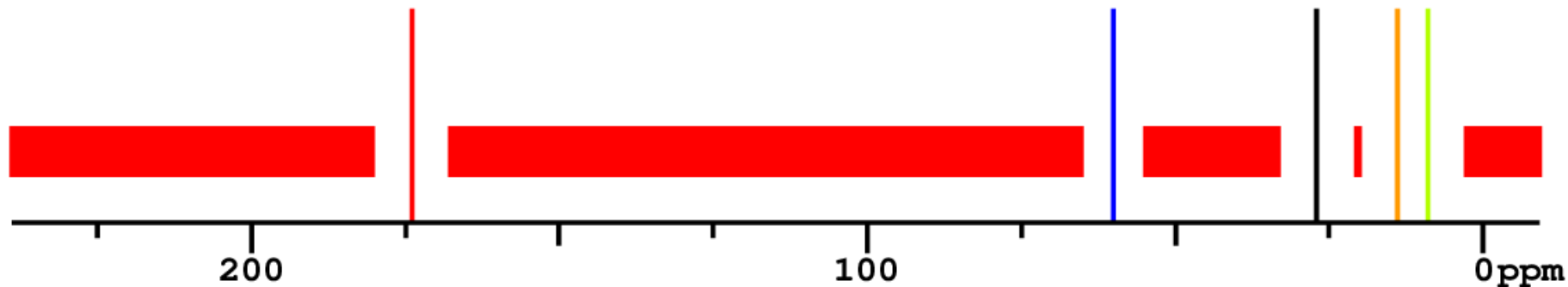
Signal multiplicity: S D T Q O E P ?





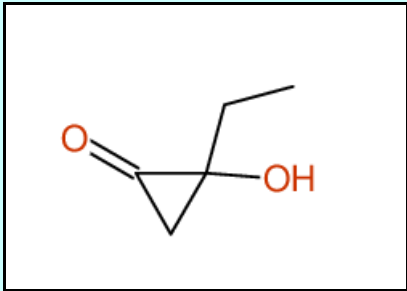
Experimental shift values

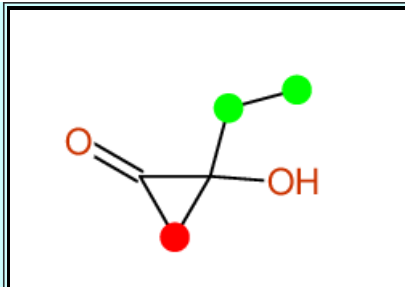
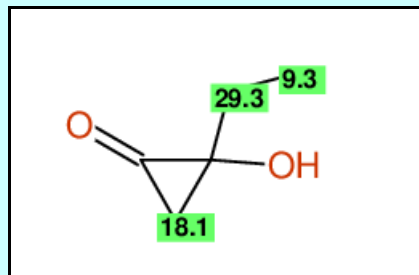
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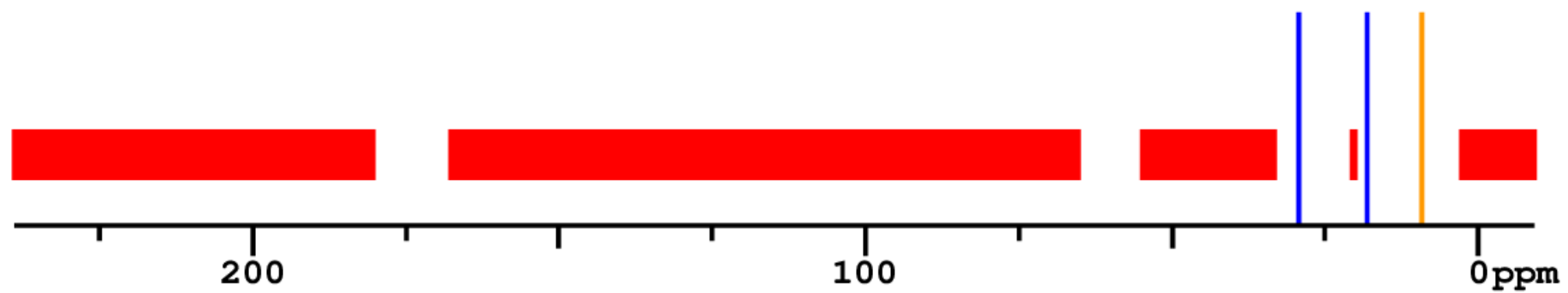
### Structure Proposal #46

Structure	Similarity Measure
	Deviation = 9.65 ppm Similarity = 67 %  C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>  MWT = 100.06 Search Web for this structure: <a href="#">GTNDLTKJPEYUJS</a>
Predicted Chemical Shiftvalues	Matching Map



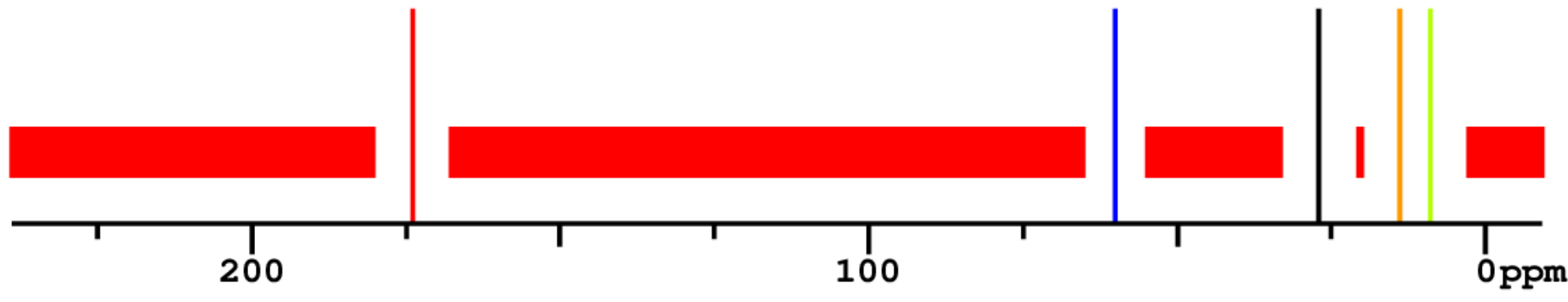
Predicted shift values

Signal multiplicity: S D T Q O E P ?



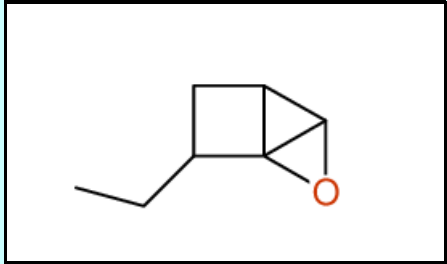
Experimental shift values

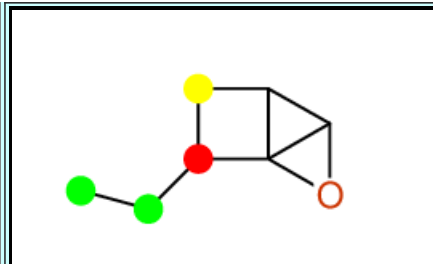
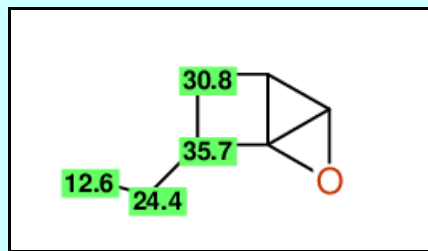
No line in reference: 



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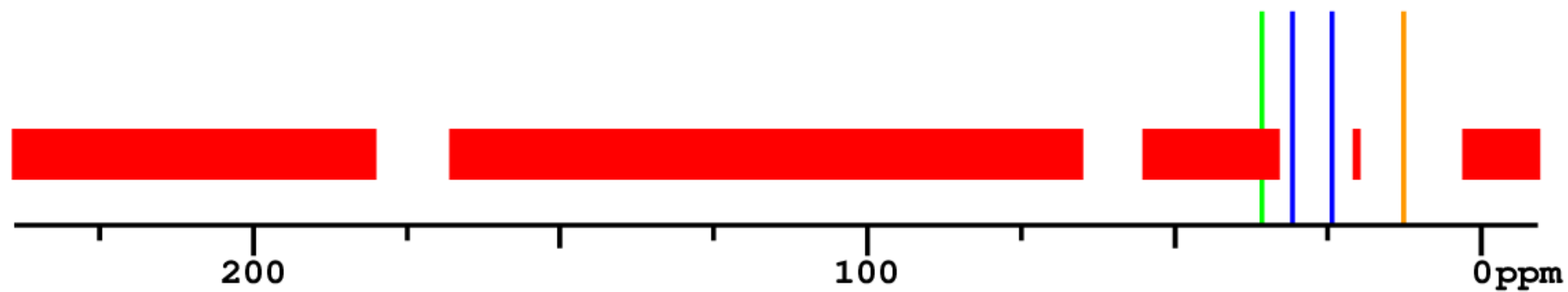
Structure Proposal #47

Structure	Similarity Measure
	<p>Deviation = 9.66 ppm Similarity = 63 % (Different pattern)</p> <p><math>C_7H_{10}O</math></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">SUBRYTRHWOBQQ!</a></p>
Predicted Chemical Shiftvalues	Matching Map



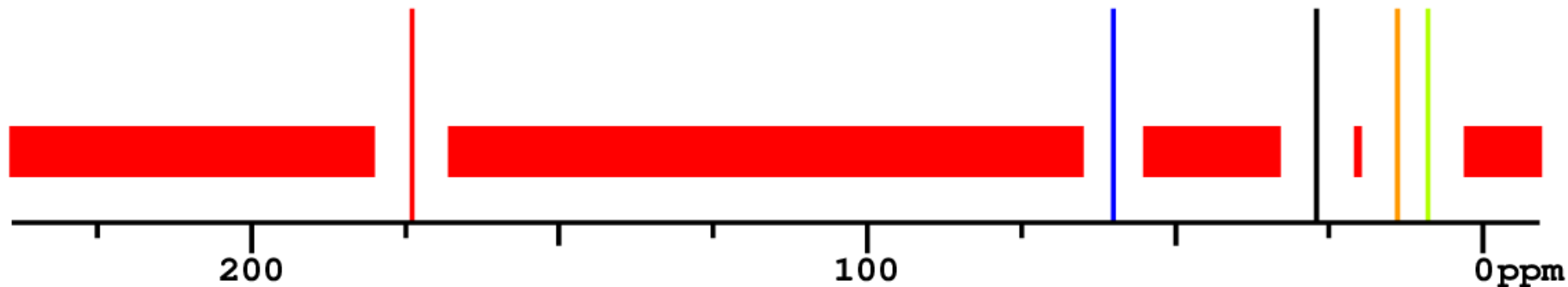
Predicted shift values

Signal multiplicity: S D T Q O E P ?



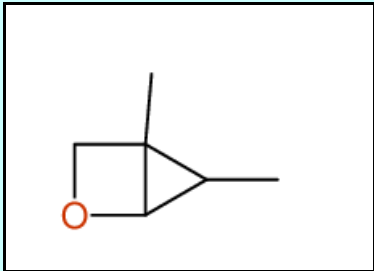
Experimental shift values

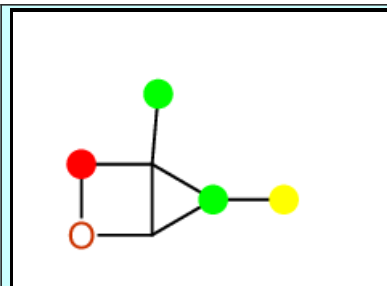
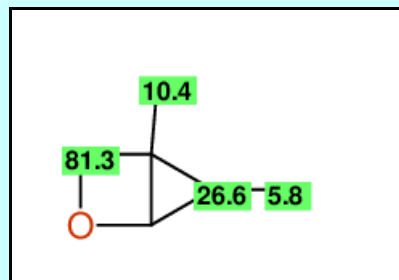
No line in reference: ████████



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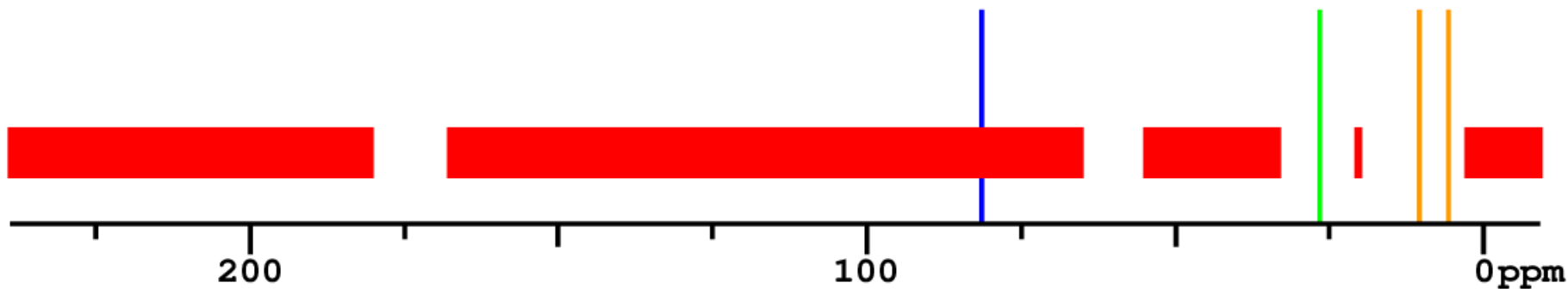
### Structure Proposal #48

Structure	Similarity Measure
	<p>Deviation = 9.71 ppm Similarity = 63 % (Different pattern)</p> <p><math>C_6H_{10}O</math></p> <p>MWT = 98.07</p> <p>Search Web for this structure: <a href="#">IPPBHXUICADJGT</a></p>
Predicted Chemical Shiftvalues	Matching Map



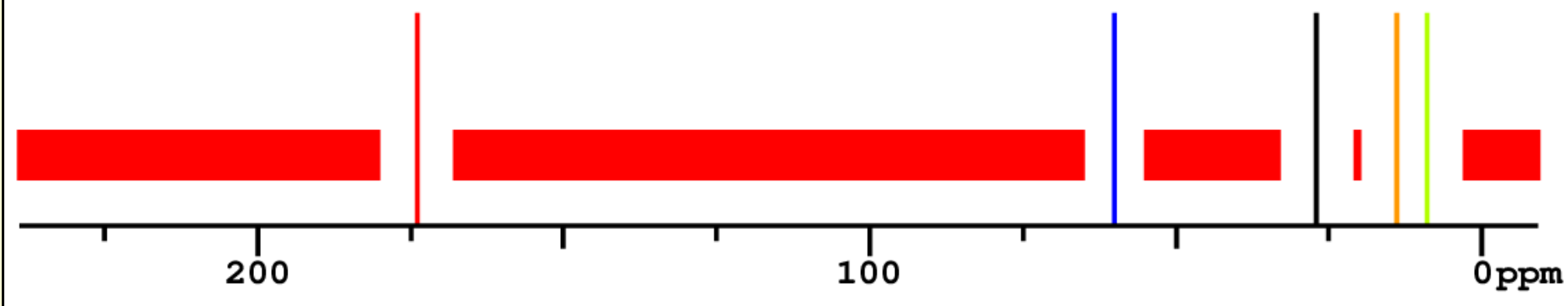
Predicted shift values

Signal multiplicity: S D T Q O E P ?



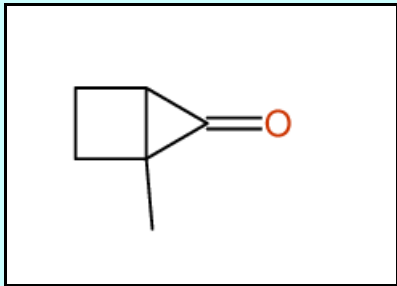
Experimental shift values

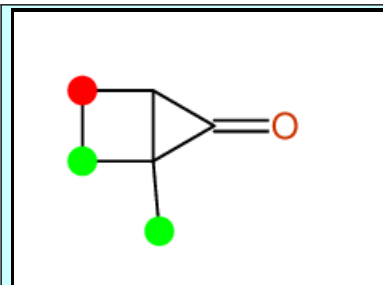
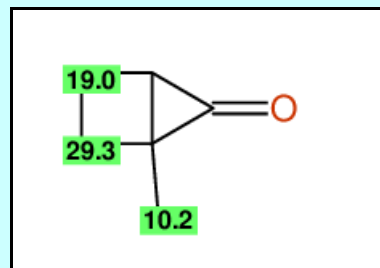
No line in reference: 



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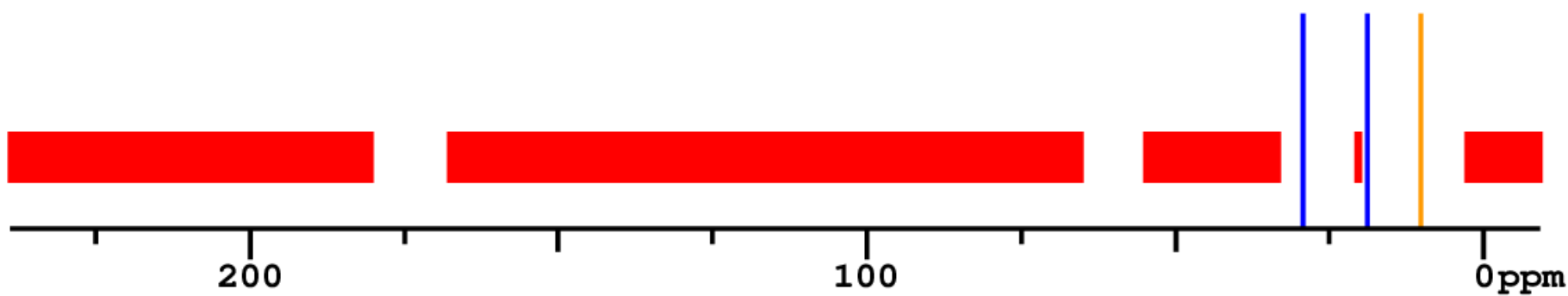
### Structure Proposal #49

Structure	Similarity Measure
	Deviation = 9.76 ppm Similarity = 67 %  $C_6H_8O$  MWT = 96.07  Search Web for this structure:  <a href="#">ORTSZQHNPUCPJW</a>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

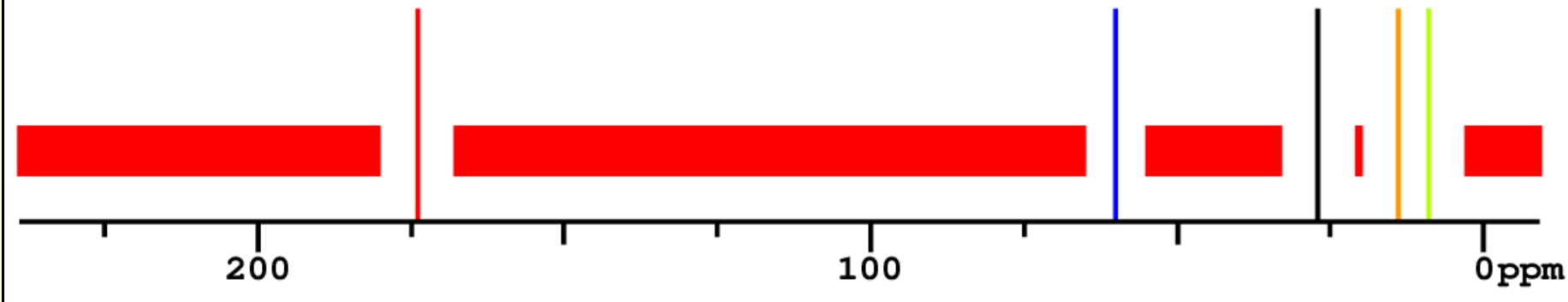
Signal multiplicity: S D T Q O E P ?





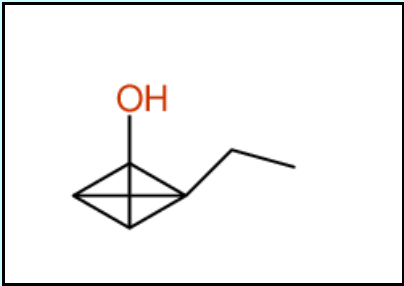
Experimental shift values

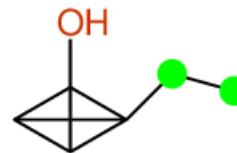
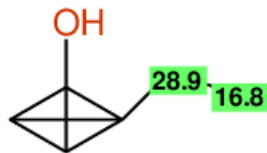
No line in reference: 



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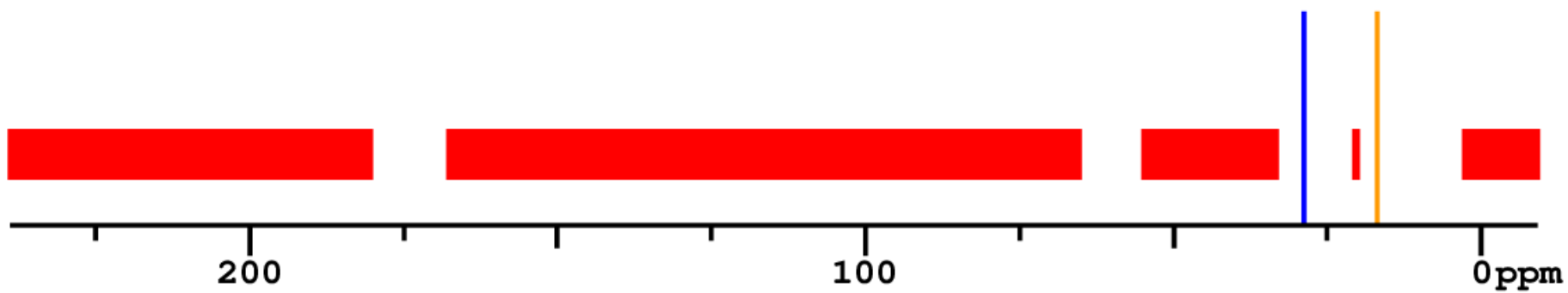
### Structure Proposal #50

Structure	Similarity Measure
	Deviation = 9.85 ppm Similarity = 100 %  C <sub>6</sub> H <sub>8</sub> O  MWT = 96.07 Search Web for this structure: <a href="#">LNUXUXAQV5IAA</a>
Predicted Chemical Shiftvalues	Matching Map



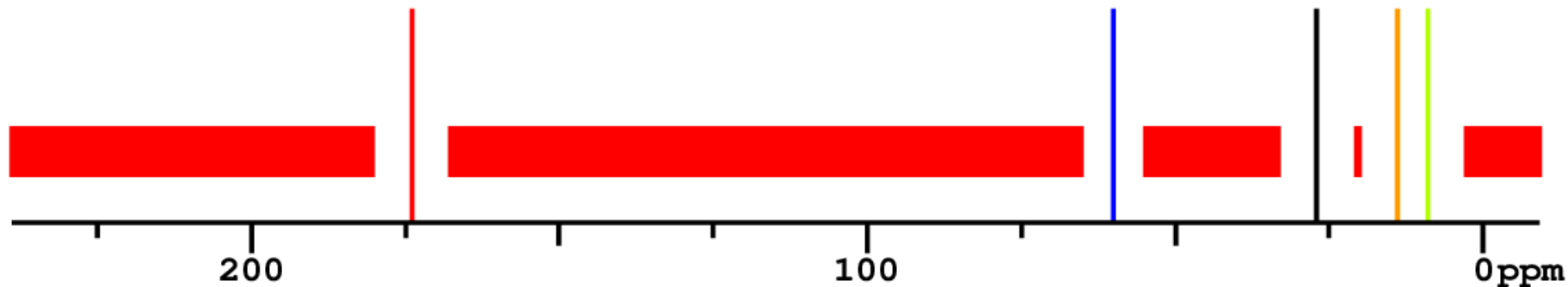
Predicted shift values

Signal multiplicity: S D T Q O E P ?



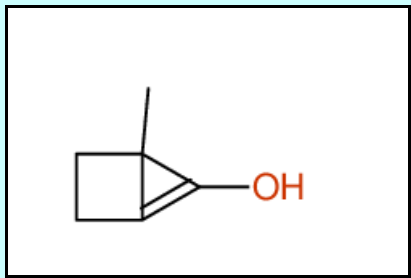
Experimental shift values

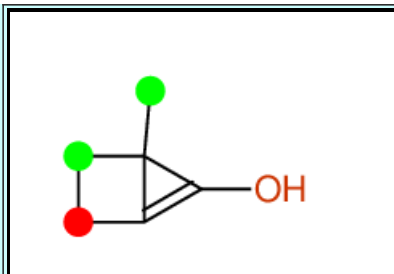
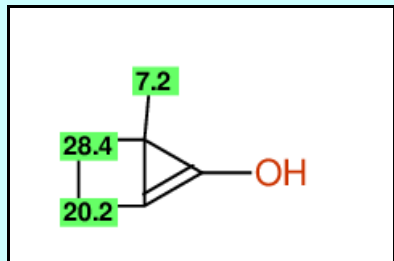
No line in reference: ████████



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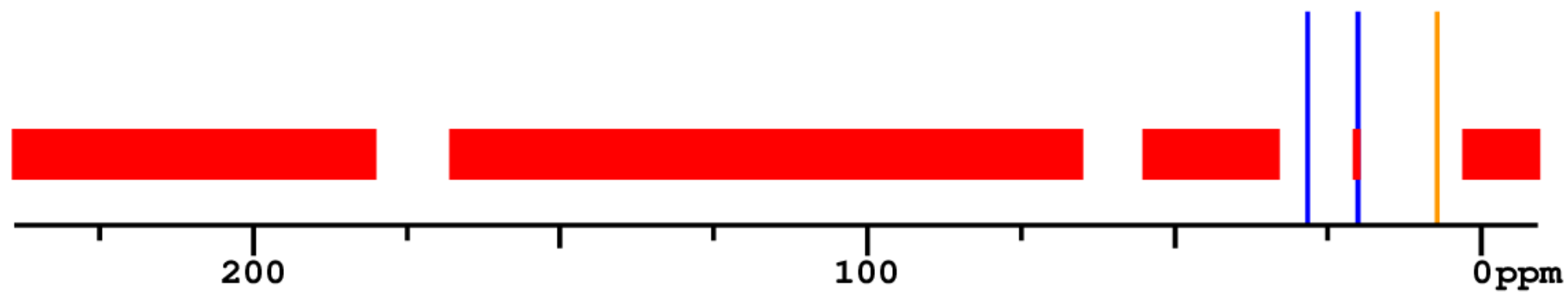
### Structure Proposal #51

Structure	Similarity Measure
	<p>Deviation = 9.91 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_8O</math></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">QNDKYNSAESMQHX</a></p>
Predicted Chemical Shiftvalues	Matching Map



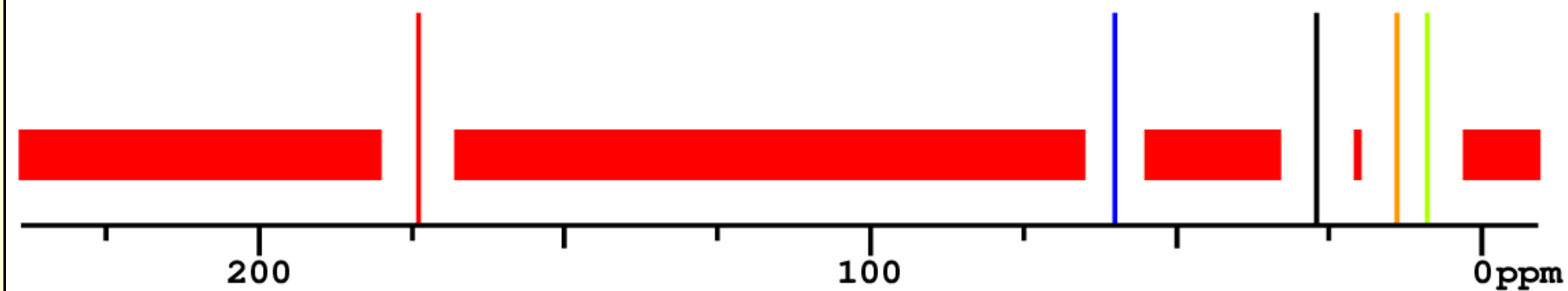
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: ████████

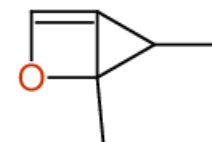


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### Summary of the 10 most frequently occurring parent ring systems within the 17 best-fitting entries

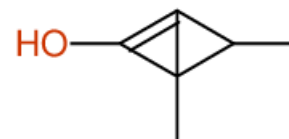
Occurence:

1 in 17



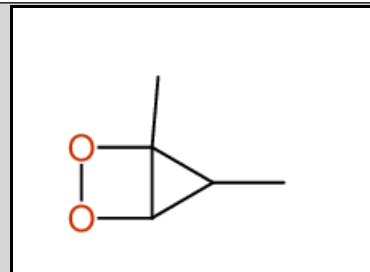
Occurence:

1 in 17



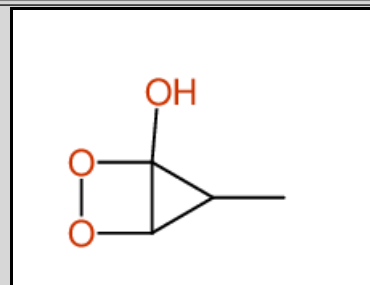
Occurence:

1 in 17



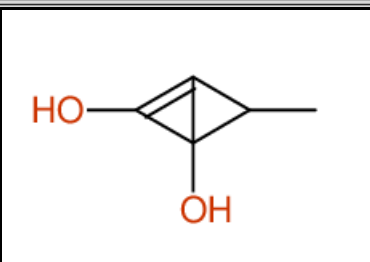
Occurence:

1 in 17



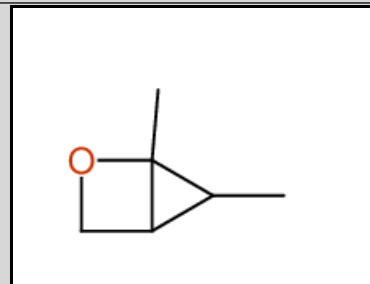
Occurence:

1 in 17



Occurence:

1 in 17



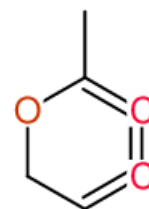
Occurrence:

1 in 17



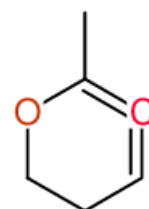
Occurrence:

1 in 17



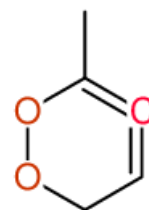
Occurrence:

1 in 17



Occurrence:

1 in 17



## Summary of Processing

Checking existence of data and counting them:	20,000,000 entries in 0.342 seconds
Applying restraints from elemental composition:	5.449 seconds, 510,515 entries remain
Applying restraints from number of signals:	0.427 seconds, 16,134 entries remain
Searching 299,998,280 chemical shift values line-per-line:	3.043 seconds
Best 2,886 entries selected for analysis:	0.466 seconds
Ranking of 2,886 entries by similarity:	29.545 seconds
Deviation of best match:	3.82 ppm
Creating table and linking 2,886 structures to 475,803 INCHIKEY-pages:	0.582 seconds
Detailed Analysis of 51 structures including graphical representation:	7.054 seconds
Analysis of 17 structures for common parent ring systems:	0.008 seconds
Total CPU-usage:	47.647 seconds
Data transferred from disk:	1,225 MBytes out of 290,546 MBytes
Program version:	20200916_2-3D-zip/00
Machine:	I9-9900K / 16x3.60GHz
<p>Page written by Wolfgang Robien using CSEARCH-Technology Page written on 2021:05:19 at 19:07 Page finished on 2021:05:19 at 19:09</p> <p>Have a nice day !</p>	