

Spectral Similarity Search based on  
**144,833,798 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 19:08

This page will be kept for 30 days here

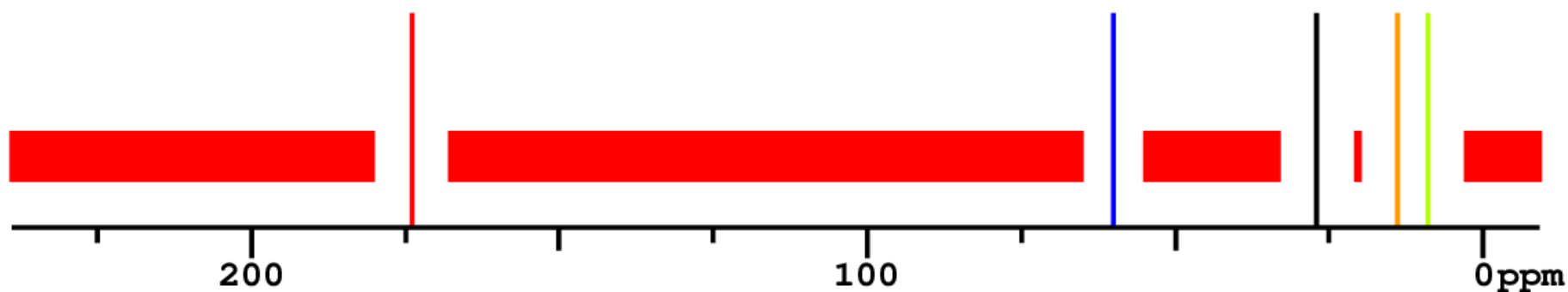
<b>Name of Project:</b>	<b>Test1</b>
<b>Comment:</b>	<b>Dereplication-engine</b>
<b>Name of Compound:</b>	<b>Propionic_acid,ethylester 400MHz</b>

### 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:	144,833,798
Compounds containing: N	137,193,882
Compounds containing: O	132,274,161
Compounds containing: P	824,792
Compounds containing: S	38,732,013
Compounds containing: F	26,618,673
Compounds containing: Cl	15,032,432
Compounds containing: Br	9,103,558
Compounds containing: I	1,175,064
Compounds containing: other	1,206,973

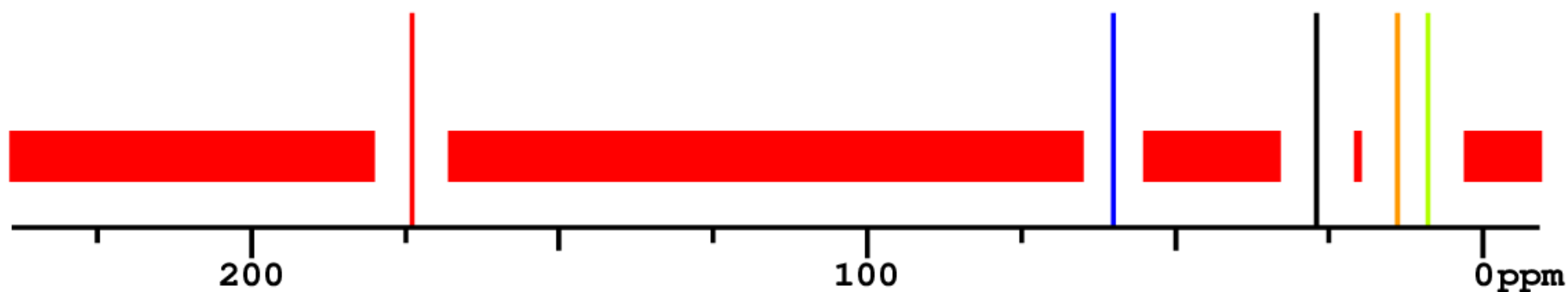
Available entries at each Screening-Step	
Total number of entries:	144,833,798

Applying requested elemental composition:	3,593,931 entries remain
Applying requested number of signals:	104,807 entries remain

Entries per line found out of 104,807 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	S	3.00	11,955	Impurity ?
2	60.00	T	2.50	10,576	Unspecific line
3	27.00	?	3.00	39,616	Unspecific line
4	14.00	Q	3.00	19,908	Unspecific line
5	9.00	P	3.00	18,395	Unspecific line

Experimental shift values

No line in reference: ████████



Number of coincident lines versus number of entries

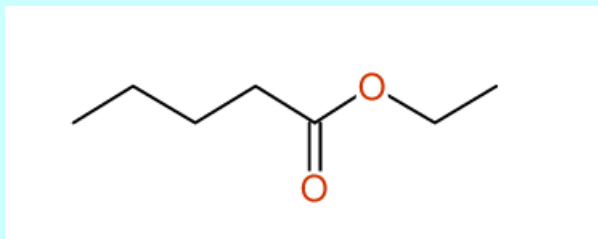
Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	21	Selected for detailed analysis
4	404	Selected for detailed analysis
3	4,228	Selected for detailed analysis
2	20,139	
1	45,767	

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

2.73 -  
2.73ppm

1x found

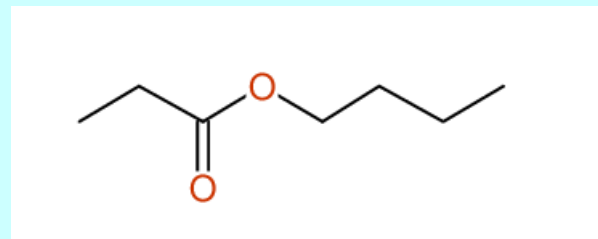
[VUXQCEFKOQTQO](#)



2.96 -  
2.96ppm

1x found

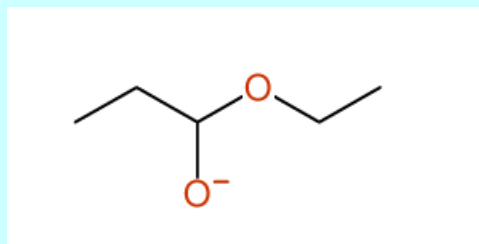
[YQKXIRZLKBWITR](#)



3.31 -  
3.31ppm

1x found

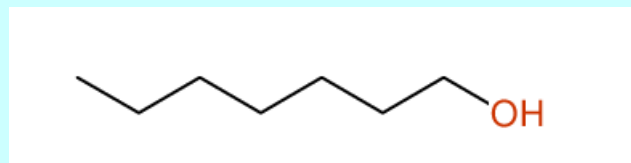
[GJYJNGCLZFAEMH](#)



3.38 -  
3.38ppm

1x found

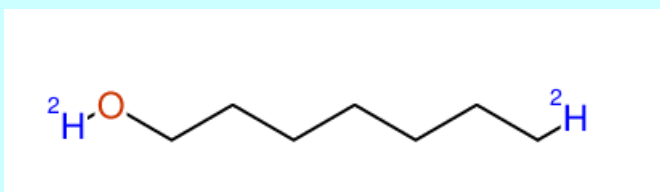
[ARYJKUMSSIOOH](#)



3.38 - 3.38ppm

1x found

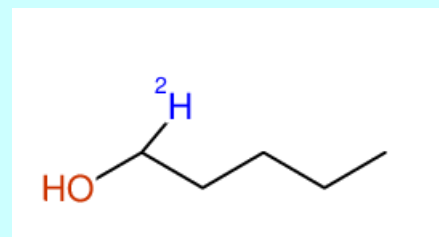
[BBMCTIGTTCKYKE](#)



3.40 -  
3.40ppm

2x found

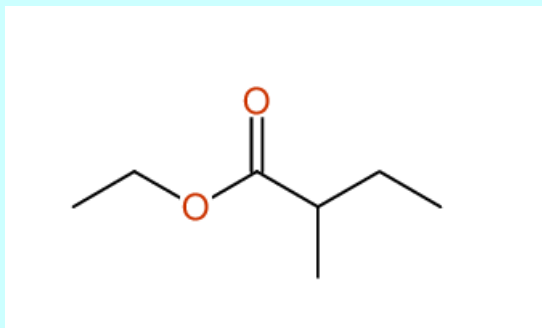
[AMQJEAYHLZJPGS](#)



3.41 -  
3.41ppm

1x found

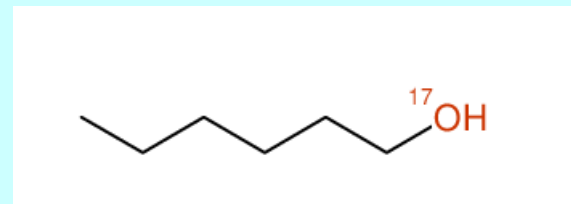
[JPVJIJBICKBKSH](#)



3.44 -  
3.44ppm

2x found

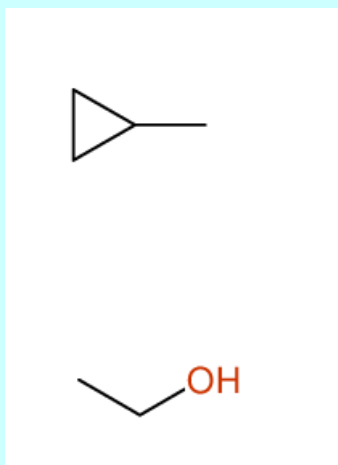
[ZSIAUFGUXNUGDI](#)



3.56 -  
3.56ppm

1x found

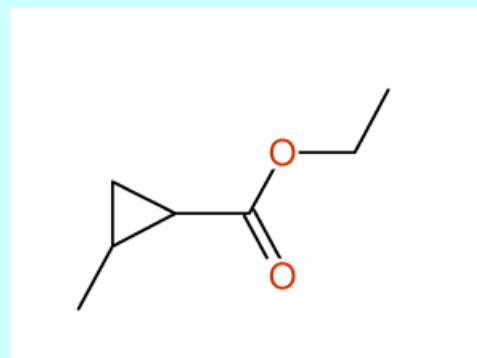
[OTVBAIYXRCXJKL](#)



3.72 -  
3.72ppm

1x found

[ZNXRPIKPYJZPNI](#)

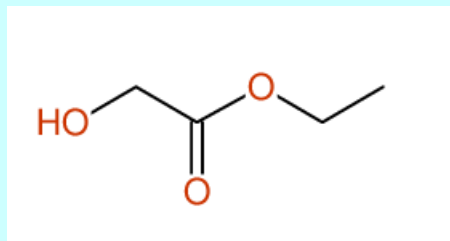




3.72 -  
3.72ppm

1x found

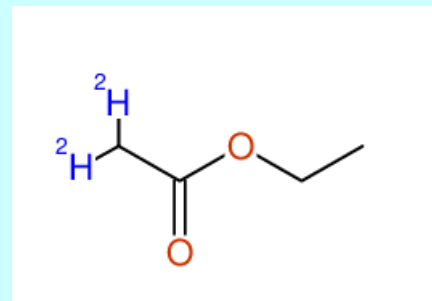
[USTOPXSKJLOMKG](#)



3.74 -  
3.74ppm

1x found

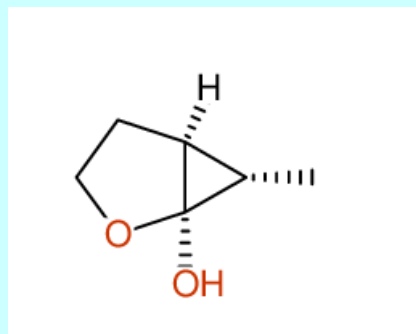
[XEKOWRVHYACXOJ](#)



3.77 -  
3.77ppm

1x found

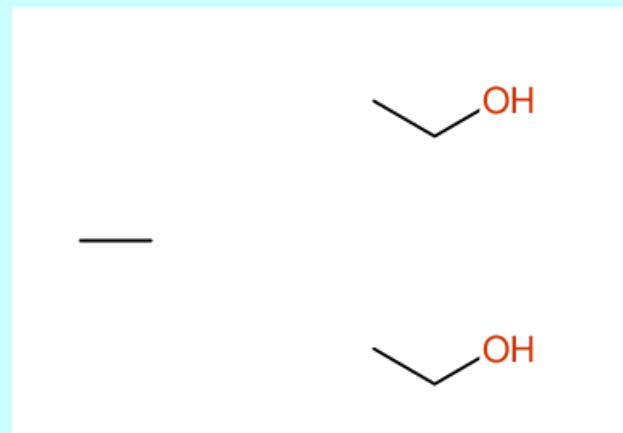
[OKQNTQARVDVCHK](#)



4.04 -  
4.04ppm

1x found

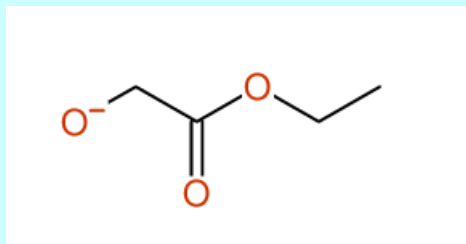
[MKNBWAXUAMKIOZ](#)



4.11 -  
4.11ppm

1x found

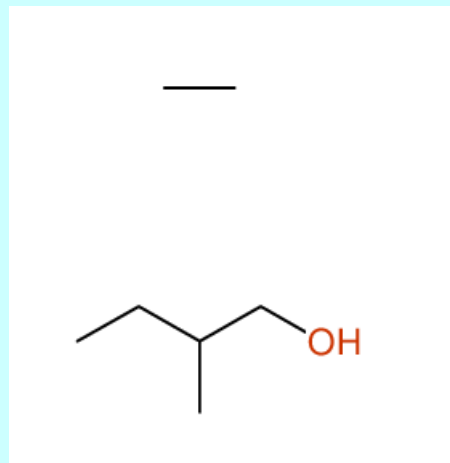
[PDHCCQJYEKLVRY](#)



4.15 -  
4.15ppm

2x found

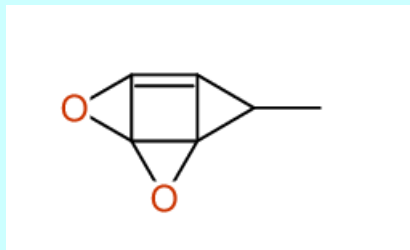
[QSLNWESTNWAUCD](#)



4.26 -  
4.26ppm

1x found

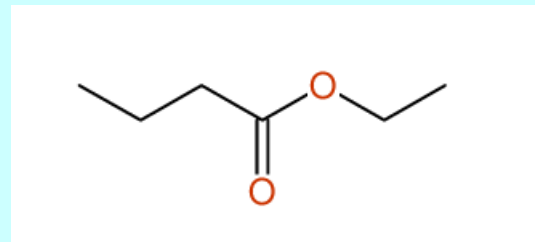
[HFYYMLXNNBCFAY](#)

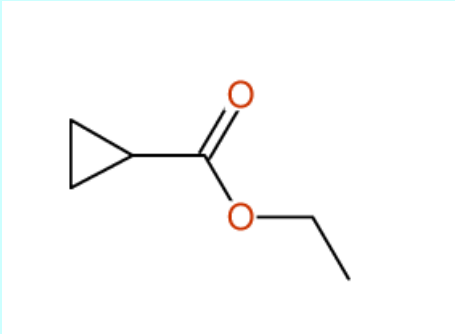
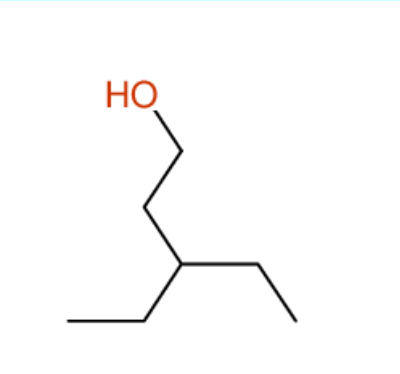


4.32 -  
4.32ppm

1x found

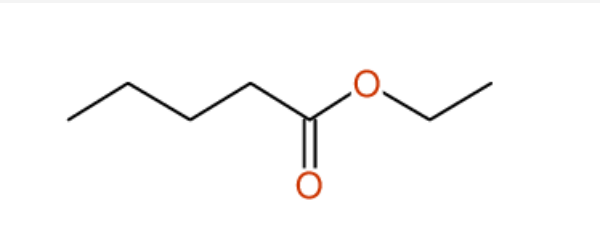
[OBNCKNCVKJNDBV](#)



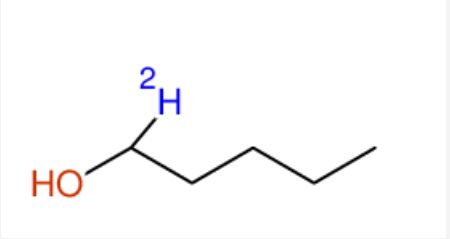

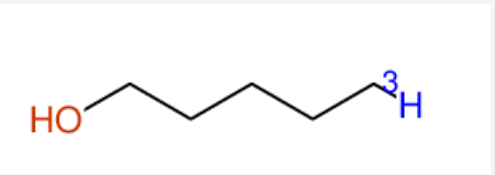

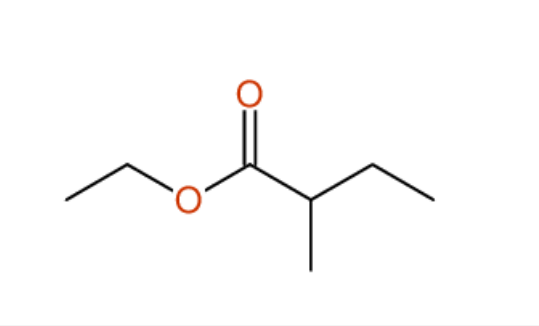
4.35 - 4.35ppm	1x found	<a href="#">OARDGAWFHAUOJC</a>	4.36 - 4.36ppm	1x found	<a href="#">RLVPCYMDLYVFHH</a>
					

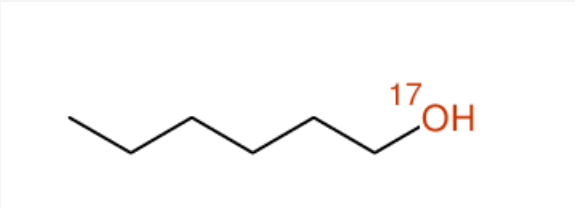

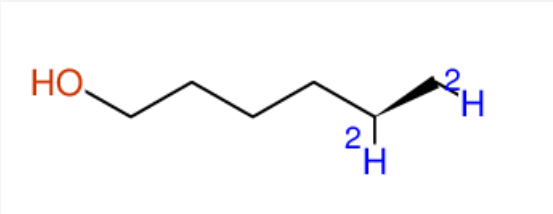

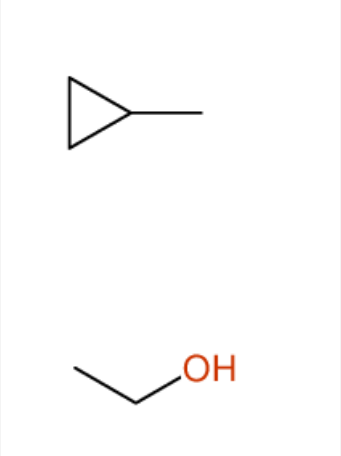
4,653 [Structure proposals](#) found for your C-NMR Spectrum

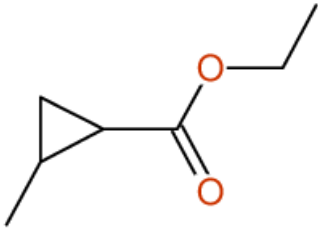
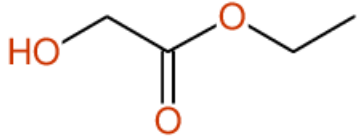
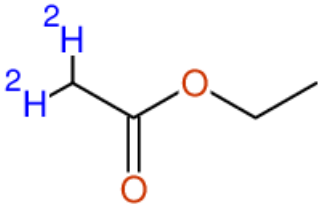

198 Entries will be shown because of your selection of additional constraints

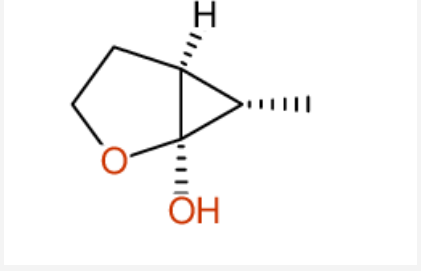
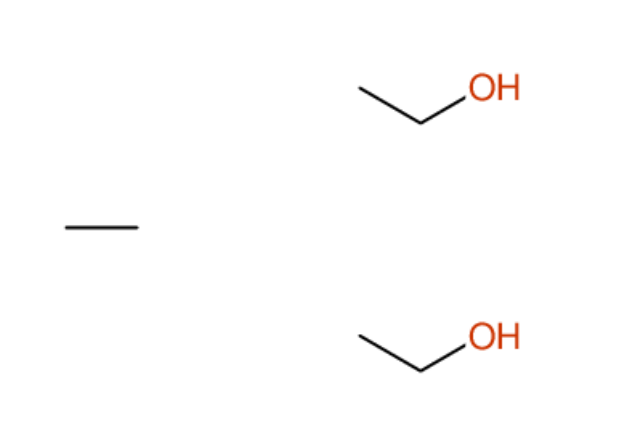
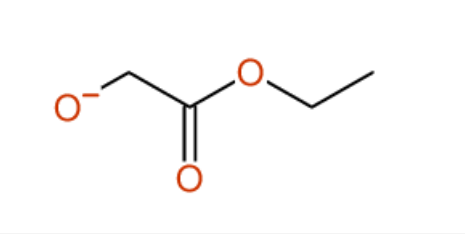
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1  2.73  <a href="#">Details</a>  Different pattern		C <sub>7</sub> O <sub>2</sub>  MWT = 116.077	Proposal #1  Structure-ID: 143,973,553  <a href="#">VUXQCEFKOQUTQO-UHFFFAOYAP</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #2  2.96  <a href="#">Details</a>  Different pattern		$C_7O_2$  MWT = 116.077	Proposal #2  Structure-ID: 143,961,843  <a href="#">YQKXIRZLKBWITR-UHFFFAOYAA</a>	
Proposal #3  3.31  <a href="#">Details</a>		$C_5H_{11}O_2$  MWT = 103.055	Proposal #3  Structure-ID: 97,520,174  <a href="#">GJYJNGCLZFAEMH-UHFFFAOYAS</a>	
Proposal #4  3.38  <a href="#">Details</a>  Different pattern		$C_7O$  MWT = 100.077	Proposal #4  Structure-ID: 106,386,740  <a href="#">ARYJKUMSSIOOH-UHFFFAOYAA</a>	
Proposal #5  3.38  <a href="#">Details</a>  Different pattern		$C_7H_{16}O$  MWT = 118.077	Proposal #5  Structure-ID: 91,945,230  <a href="#">BBMCTIGTCKYKE-NRIOPPFLEB</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  

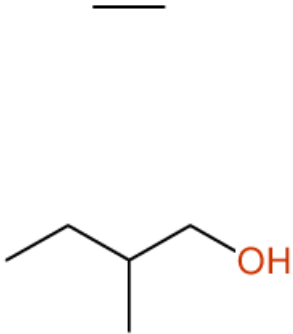
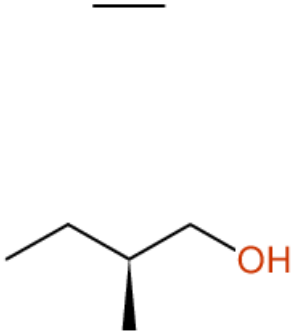
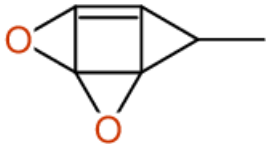
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #6  3.40  <a href="#">Details</a>		$C_5H_{12}O$ MWT = 89.055	Proposal #6 Structure-ID: 63,686,477 <a href="#">AMQJEAYHLZJPGS-UICOGKGYEB</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH 
Proposal #7  3.40  <a href="#">Details</a>		$C_5H_{12}O$ MWT = 90.055	Proposal #7 Structure-ID: 92,976,292 <a href="#">AMQJEAYHLZJPGS-CNRUNOGKEA</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH 
Proposal #8  3.41  <a href="#">Details</a>  Different pattern		$C_7O_2$ MWT = 116.077	Proposal #8 Structure-ID: 106,480,336 <a href="#">JPVJIJBICKBKSH-UHFFFAOYAB</a>	

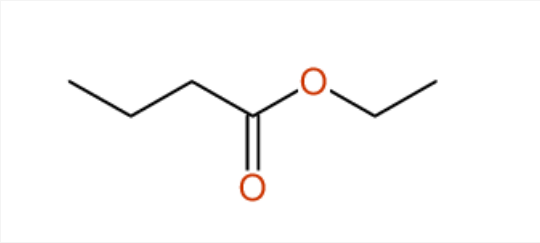

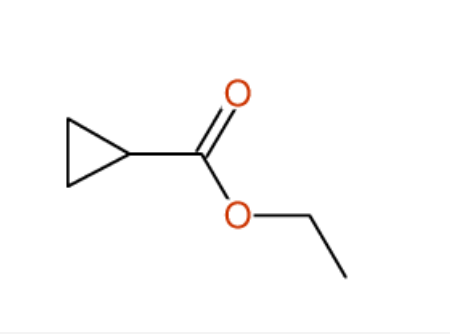
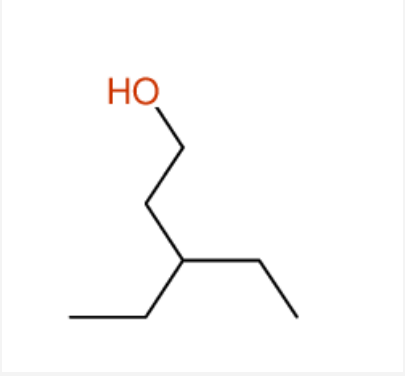
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #9</p> <p>3.44</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{14}O</math></p> <p>MWT = 103.066</p>	<p>Proposal #9</p> <p>Structure-ID: 97,555,684</p> <p><a href="#">ZSIAUFGUXNUGDI-CDZYAPPEA</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #10</p> <p>3.44</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{14}O</math></p> <p>MWT = 104.066</p>	<p>Proposal #10</p> <p>Structure-ID: 97,555,685</p> <p><a href="#">ZSIAUFGUXNUGDI-XVUBXAANFC</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #11</p> <p>3.56</p> <p><a href="#">Details</a></p>		<p><math>C_4H_8 \cdot C_2H_6O</math></p> <p>MWT = 102.066</p>	<p>Proposal #11</p> <p>Structure-ID: 41,693,659</p> <p><a href="#">OTVBAIYXRCXJKL-UHFFFAOYAP</a></p>	

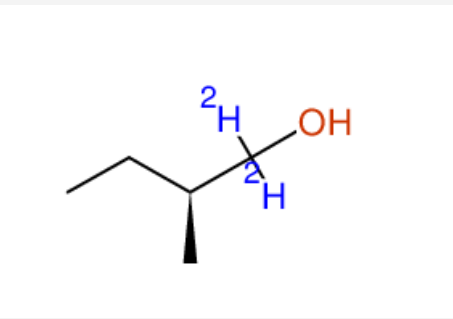

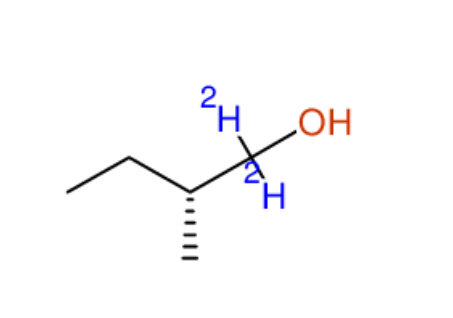

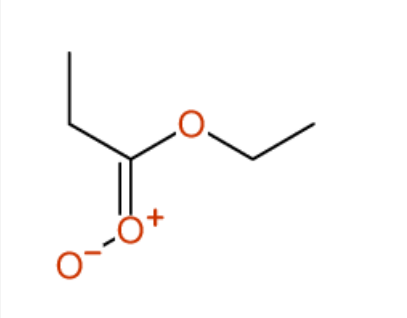
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #12  3.72  <a href="#">Details</a>		$C_7O_2$ MWT = 116.077	Proposal #12 Structure-ID: 143,974,183 <a href="#">ZNXRPIKPYJZPNI-UHFFFAOYAZ</a>	
Proposal #13  3.72  <a href="#">Details</a>		$C_4O_3$ MWT = 96.044	Proposal #13 Structure-ID: 143,973,744 <a href="#">USTOPXSKJLOMKG-UHFFFAOYAE</a>	
Proposal #14  3.74  <a href="#">Details</a>  Different pattern		$C_4H_8O_2$ MWT = 90.044	Proposal #14 Structure-ID: 92,737,183 <a href="#">XEKOWRVHYACXOJ-CBTSVUPCEF</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  

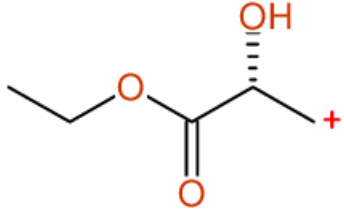
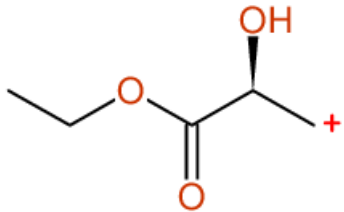
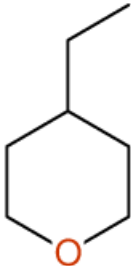
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #15</p> <p>3.77</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.066</p>	<p>Proposal #15</p> <p>Structure-ID: 93,348,236</p> <p><a href="#">OKQNTQARVDVCHK-HCWXCVPGBN</a></p>	
<p>Proposal #16</p> <p>4.04</p> <p><a href="#">Details</a></p>		<p><math>2C_2H_6O.C_2H_6</math></p> <p>MWT = 116.066</p>	<p>Proposal #16</p> <p>Structure-ID: 41,377,361</p> <p><a href="#">MKNBWAXUAMKIOZ-UHFFFAOYAP</a></p>	
<p>Proposal #17</p> <p>4.11</p> <p><a href="#">Details</a></p>		<p><math>C_4H_7O_2</math></p> <p>MWT = 103.044</p>	<p>Proposal #17</p> <p>Structure-ID: 98,518,941</p> <p><a href="#">PDHCCQJYEKLVRY-UHFFFAOYAC</a></p>	

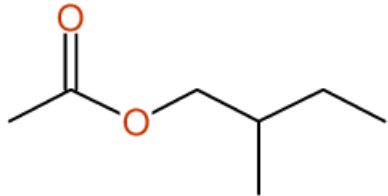
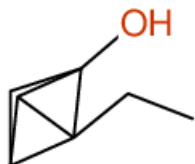
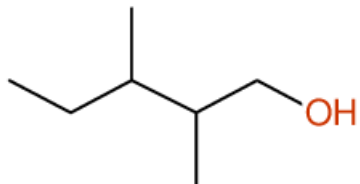
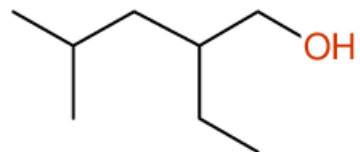


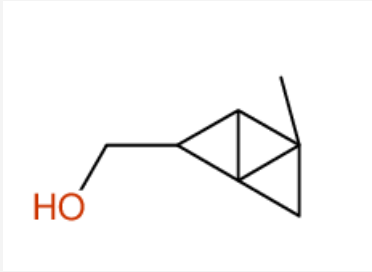
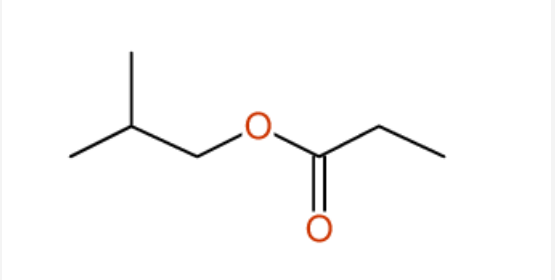
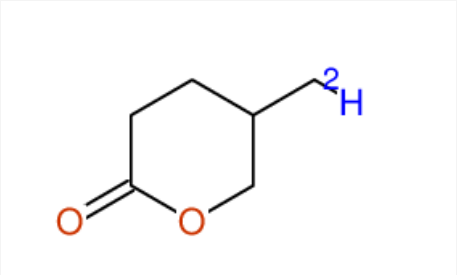

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #18  4.15 <a href="#">Details</a> Different pattern		$C_5H_{12}O \cdot C_2H_6$ MWT = 118.077	Proposal #18 Structure-ID: 37,508,796 <a href="#">QSLNWESTNVAWCD-UHFFFAOYAW</a>	
Proposal #19  4.15 <a href="#">Details</a> Different pattern		$C_5H_{12}O \cdot C_2H_6$ MWT = 118.077	Proposal #19 Structure-ID: 17,729,712 <a href="#">QSLNWESTNVAWCD-JEDNCBNOBQ</a>	
Proposal #20  4.26 <a href="#">Details</a>		$C_6H_4O_2$ MWT = 108.066	Proposal #20 Structure-ID: 74,403,615 <a href="#">HFYYMLXNNBCFAY-UHFFFAOYAT</a>	

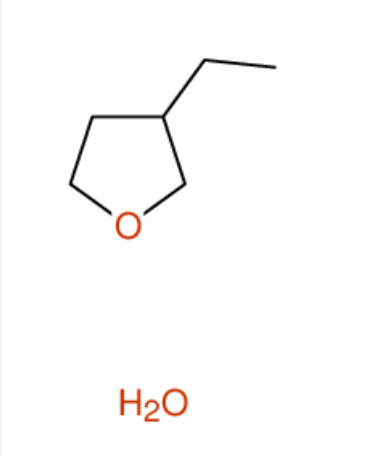
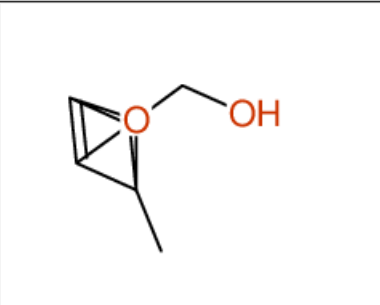
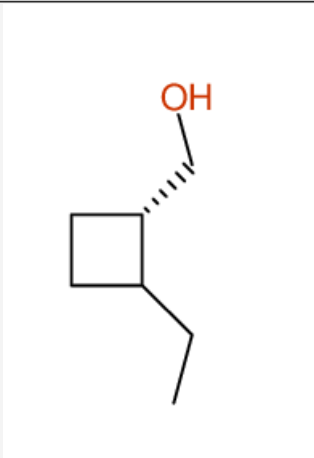
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #21  4.32  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$  MWT = 116.066	Proposal #21  Structure-ID: 135,913,890  <a href="#">OBNCKNCVKJNDBV-IKLDFBCSAI</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  
Proposal #22  4.35  <a href="#">Details</a>		$C_6O_2$  MWT = 104.066	Proposal #22  Structure-ID: 143,974,802  <a href="#">OARDGAWFHAUOJC-UHFFFAOYAC</a>	
Proposal #23  4.36  <a href="#">Details</a>  Different pattern		$C_7O$  MWT = 100.077	Proposal #23  Structure-ID: 144,037,500  <a href="#">RLVPCYMDLYVFHH-UHFFFAOYAF</a>	

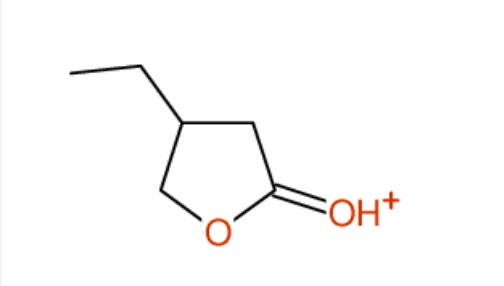

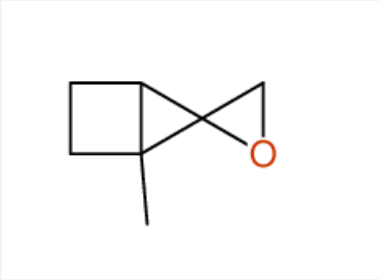
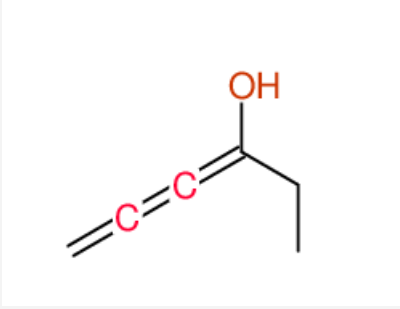
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #24</p> <p>4.42</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_{12}O</math></p> <p>MWT = 90.055</p>	<p>Proposal #24</p> <p>Structure-ID: 18,350,514</p> <p><a href="#">QPRQEDXDYOZYLA-HUFQHLJSFU</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #25</p> <p>4.42</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_5H_{12}O</math></p> <p>MWT = 90.055</p>	<p>Proposal #25</p> <p>Structure-ID: 18,350,551</p> <p><a href="#">QPRQEDXDYOZYLA-IEJGYHECFL</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #26</p> <p>4.61</p> <p><a href="#">Details</a></p>		<p><math>C_5H_{10}O_3</math></p> <p>MWT = 118.055</p>	<p>Proposal #26</p> <p>Structure-ID: 38,644,338</p> <p><a href="#">DIYGJYIIGSAVGQ-UHFFFAOYAE</a></p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #27</p> <p>4.70</p> <p><a href="#">Details</a></p>		<p><math>C_5H_9O_3</math></p> <p>MWT = 117.055</p>	<p>Proposal #27</p> <p>Structure-ID: 90,719,746</p> <p><a href="#">SFMRLHJNHWEFDX-SCSAIBSYBB</a></p>	
<p>Proposal #28</p> <p>4.70</p> <p><a href="#">Details</a></p>		<p><math>C_5H_9O_3</math></p> <p>MWT = 117.055</p>	<p>Proposal #28</p> <p>Structure-ID: 90,719,745</p> <p><a href="#">SFMRLHJNHWEFDX-BYPYZUCNBM</a></p>	
<p>Proposal #29</p> <p>4.72</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_7H_{14}O.H_2</math></p> <p>MWT = 116.077</p>	<p>Proposal #29</p> <p>Structure-ID: 103,071,913</p> <p><a href="#">JWWYVYXWJOYSH-UHFFFAOYAW</a></p>	

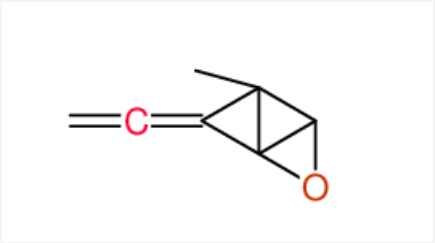
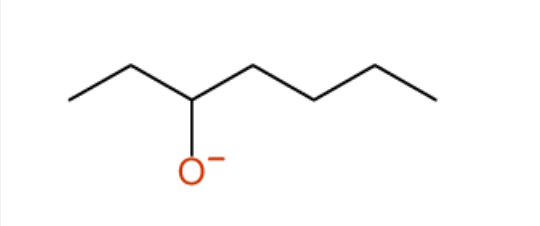
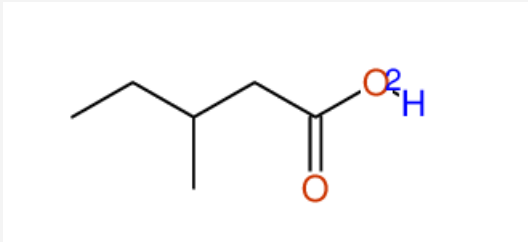
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #30  4.75  <a href="#">Details</a>  Different pattern		$C_7O_2$  MWT = 116.077	Proposal #30  Structure-ID: 106,478,409  <a href="#">APXBKUAJSWJTRL-UHFFFAOYAX</a>	
Proposal #31  4.94  <a href="#">Details</a>		$C_7H_{10}O$  MWT = 110.077	Proposal #31  Structure-ID: 120,038,460  <a href="#">JVMWIFFWQQZRFC-UHFFFAOYAG</a>	
Proposal #32  5.20  <a href="#">Details</a>  Different pattern		$C_7O$  MWT = 100.077	Proposal #32  Structure-ID: 143,974,237  <a href="#">UUESVNYVWMCSAS-UHFFFAOYAO</a>	
Proposal #33  5.49  <a href="#">Details</a>  Different pattern		$C_8O$  MWT = 112.088	Proposal #33  Structure-ID: 106,505,311  <a href="#">IDWODMMAHQBYRU-UHFFFAOYAG</a>	

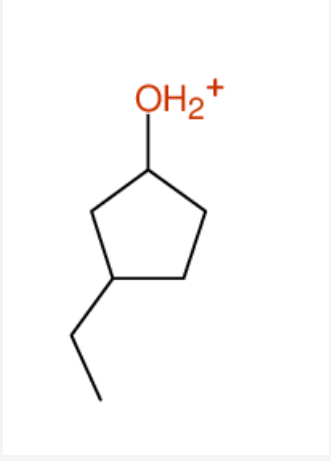
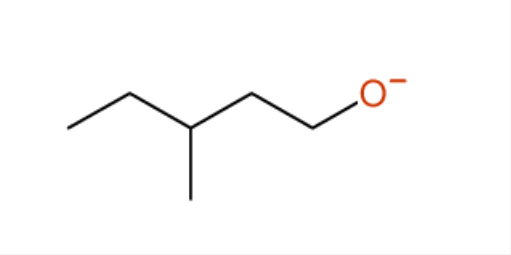
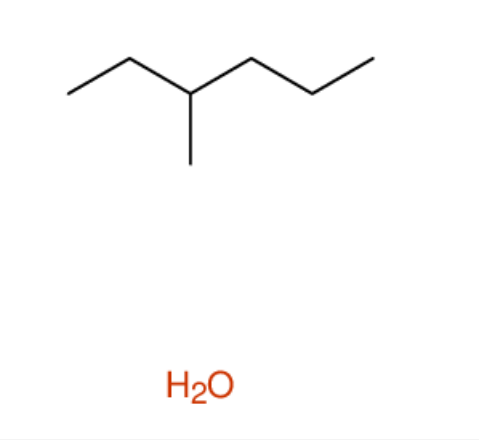
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #34</p> <p>5.60</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_7H_{10}O</math></p> <p>MWT = 110.077</p>	<p>Proposal #34</p> <p>Structure-ID: 78,257,477</p> <p><a href="#">JYMZYTRPGHEQSC-UHFFFAOYAP</a></p>	
<p>Proposal #35</p> <p>5.66</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_7O_2</math></p> <p>MWT = 116.077</p>	<p>Proposal #35</p> <p>Structure-ID: 106,489,920</p> <p><a href="#">CPOGEOGDMOTURU-UHFFFAOYAN</a></p>	
<p>Proposal #36</p> <p>5.85</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{10}O_2</math></p> <p>MWT = 115.066</p>	<p>Proposal #36</p> <p>Structure-ID: 99,656,932</p> <p><a href="#">GQUBDAOKWZLWDI-MICDWDOJER</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 

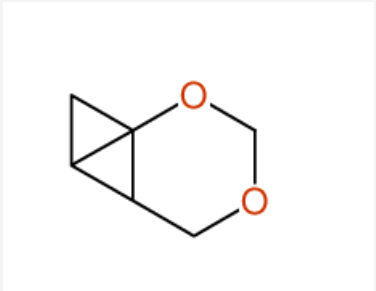
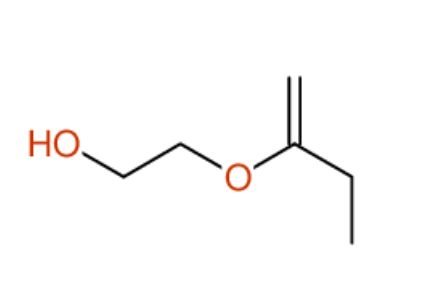
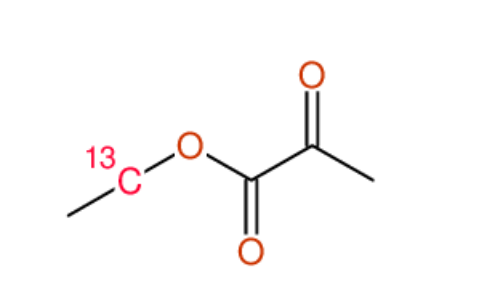

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #37</p> <p>6.27</p> <p><a href="#">Details</a></p> <p>Different pattern</p>	 <p style="text-align: center;">H<sub>2</sub>O</p>	<p>C<sub>6</sub>H<sub>12</sub>O.H<sub>2</sub>O</p> <p>MWT = 118.066</p>	<p>Proposal #37</p> <p>Structure-ID: 21,946,332</p> <p><a href="#">RSKFUFGFOZQDHE-UHFFFAOYAR</a></p>	
<p>Proposal #38</p> <p>6.35</p> <p><a href="#">Details</a></p>		<p>C<sub>6</sub>H<sub>6</sub>O<sub>2</sub></p> <p>MWT = 110.066</p>	<p>Proposal #38</p> <p>Structure-ID: 120,038,265</p> <p><a href="#">ISLZYQGILDDIOB-UHFFFAOYAB</a></p>	
<p>Proposal #39</p> <p>6.64</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p>C<sub>7</sub>H<sub>14</sub>O</p> <p>MWT = 114.077</p>	<p>Proposal #39</p> <p>Structure-ID: 99,855,090</p> <p><a href="#">HWPQBLRHKPOPJG-COBESHVIPBX</a></p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #40  6.69 <a href="#">Details</a> Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #40 Structure-ID: 93,001,017 <a href="#">MDQZVJSUBKPTHG-IKLDFFBCSAV</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  
Proposal #41  6.75 <a href="#">Details</a> Different pattern		$C_7H_{10}O$ MWT = 110.077	Proposal #41 Structure-ID: 120,036,874 <a href="#">LIKWSDHCOZEJBT-UHFFFAOYAM</a>	
Proposal #42  6.91 <a href="#">Details</a> Different pattern		$C_6H_8O$ MWT = 96.066	Proposal #42 Structure-ID: 119,846,386 <a href="#">XFXVNBAJTJGVQJ-UHFFFAOYAG</a>	



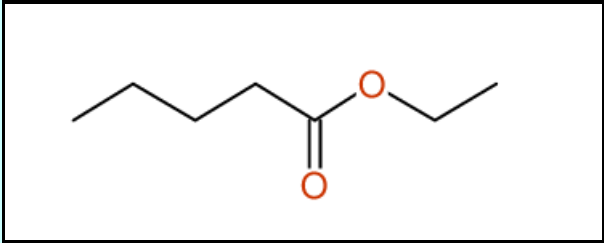
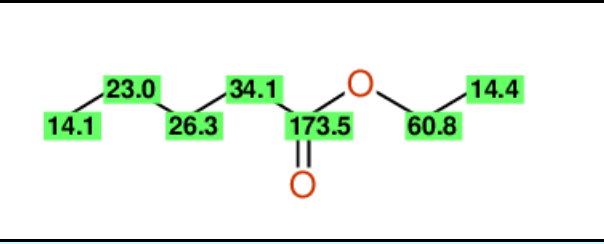
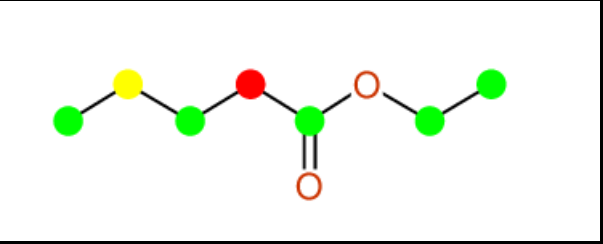
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #43  7.38  <a href="#">Details</a>  Different pattern		$C_7H_6O$  MWT = 106.077	Proposal #43  Structure-ID: 119,916,392  <a href="#">JVINKFDAUHAPDF-UHFFFAOYAC</a>	
Proposal #44  7.72  <a href="#">Details</a>  Different pattern		$C_7H_{15}O$  MWT = 115.077	Proposal #44  Structure-ID: 92,967,569  <a href="#">ORSCOPLJPMQZHQ-UHFFFAOYAM</a>	
Proposal #45  7.90  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$  MWT = 117.066	Proposal #45  Structure-ID: 93,937,090  <a href="#">IGIDLTISMCAULB-DYCDLGHIEQ</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #46</p> <p>8.04</p> <p><a href="#">Details</a></p> <p>Different pattern</p>	 <p>The structure shows a five-membered cyclopentane ring with an ethyl group (-CH<sub>2</sub>-CH<sub>3</sub>) attached to one carbon and a hydroxyl group (-OH<sub>2</sub><sup>+</sup>) attached to the adjacent carbon.</p>	<p>C<sub>7</sub>H<sub>14</sub>O</p> <p>MWT = 114.077</p>	<p>Proposal #46</p> <p>Structure-ID: 95,578,868</p> <p><a href="#">CRHZGBUSTWVQAQ-IKLDFFCSAT</a></p>	
<p>Proposal #47</p> <p>8.12</p> <p><a href="#">Details</a></p> <p>Different pattern</p>	 <p>The structure shows a four-carbon chain with a methyl group on the second carbon and an oxygen atom with a negative charge (-O<sup>-</sup>) at the end of the chain.</p>	<p>C<sub>6</sub>H<sub>13</sub>O</p> <p>MWT = 101.066</p>	<p>Proposal #47</p> <p>Structure-ID: 96,226,460</p> <p><a href="#">PMTZOPAULJSVJK-UHFFFAOYAD</a></p>	
<p>Proposal #48</p> <p>8.21</p> <p><a href="#">Details</a></p> <p>Different pattern</p>	 <p>The structure shows a five-carbon alkane chain with a methyl group on the second carbon.</p> <p>H<sub>2</sub>O</p>	<p>C<sub>7</sub>H<sub>16</sub>·H<sub>2</sub>O</p> <p>MWT = 118.077</p>	<p>Proposal #48</p> <p>Structure-ID: 20,701,145</p> <p><a href="#">GGYAZFDJULRYKQ-UHFFFAOYAJ</a></p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #49  8.39  <a href="#">Details</a>  Different pattern		$C_6H_8O_2$  MWT = 112.066	Proposal #49  Structure-ID: 120,416,208  <a href="#">VOOBIWANMYOOKZ-UHFFFAOYAV</a>	
Proposal #50  8.56  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$  MWT = 116.066	Proposal #50  Structure-ID: 71,728,946  <a href="#">XCNGAPQCDVGISX-UHFFFAOYAF</a>	
Proposal #51  8.81  <a href="#">Details</a>  Different pattern		$C_5H_8O_3$  MWT = 117.055	Proposal #51  Structure-ID: 97,582,760  <a href="#">XXRCUYVCPSWGCC-LBPDFUHNEJ</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  

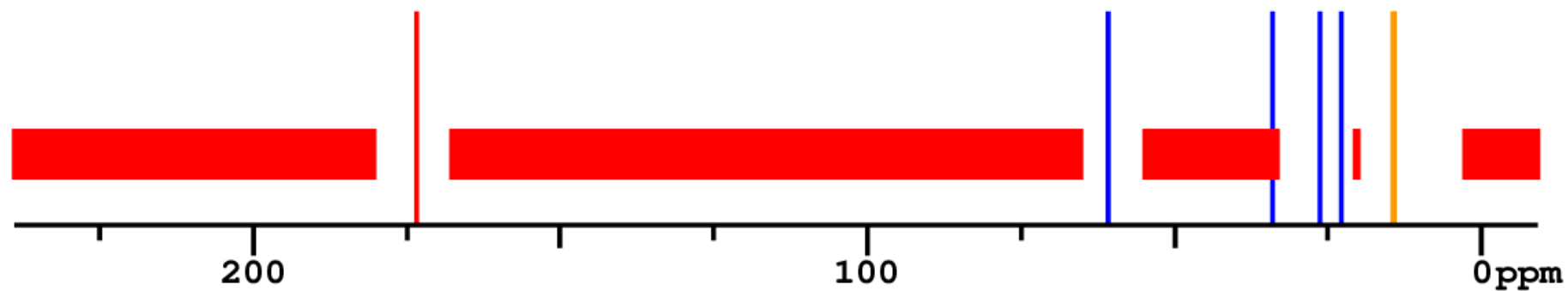
### Detailed Analysis

## Structure Proposal #1

Structure	Similarity Measure
	<p>Deviation = 2.73 ppm                      Similarity = 79 %                      (Different pattern)</p> <p><math>C_7O_2</math></p> <p>MWT = 116.08</p> <p>Search Web for this structure:  <a href="#">VUXQCFKQOUTQO</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

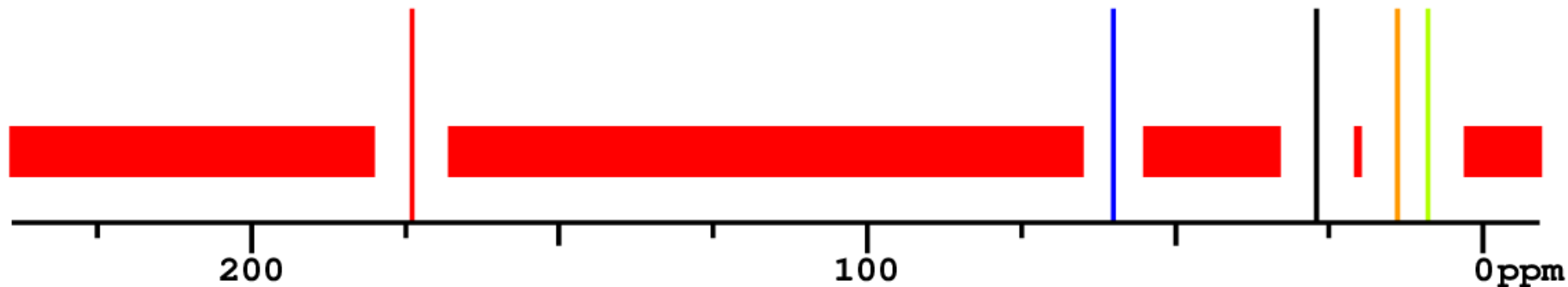
Predicted shift values

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



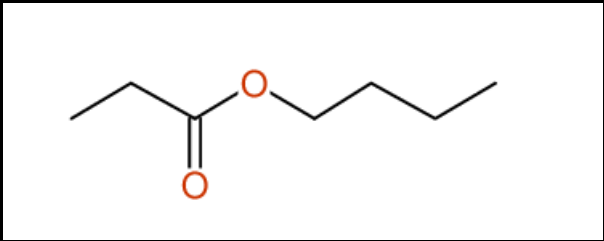
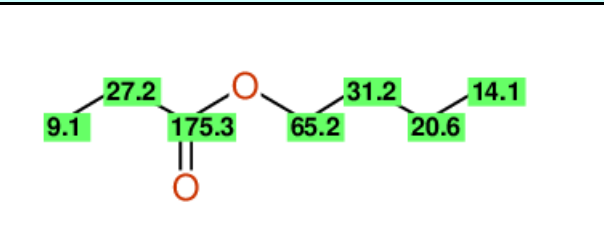
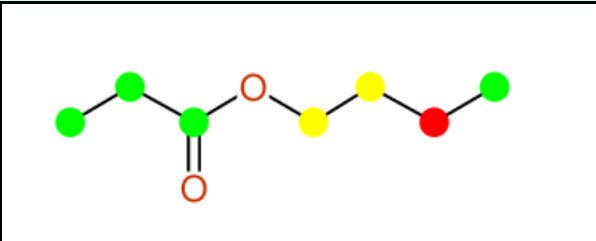
Experimental shift values

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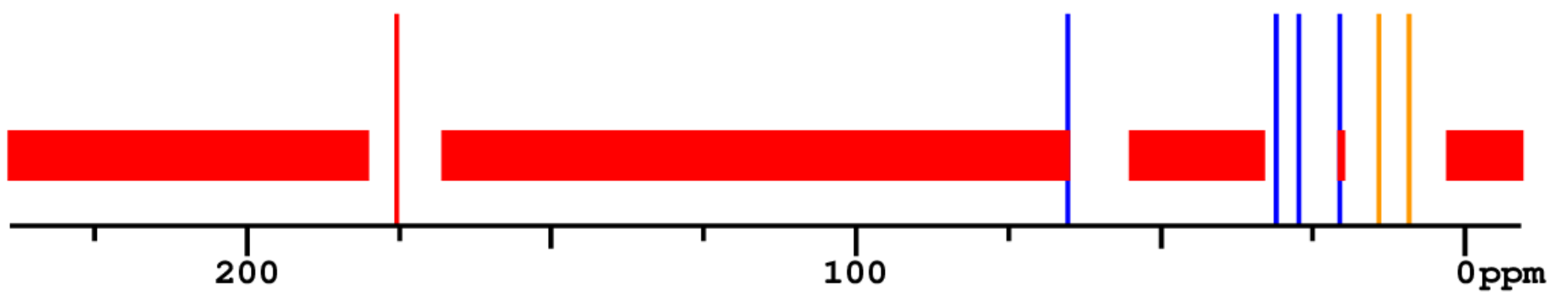
[Back to Complete Result](#)

### Structure Proposal #2

Structure	Similarity Measure
	<p>Deviation = 2.96 ppm Similarity = 71 % (Different pattern)</p> <p><math>C_7O_2</math></p> <p>MWT = 116.08</p> <p>Search Web for this structure: <a href="#">YQKXIRZLKBWTR</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

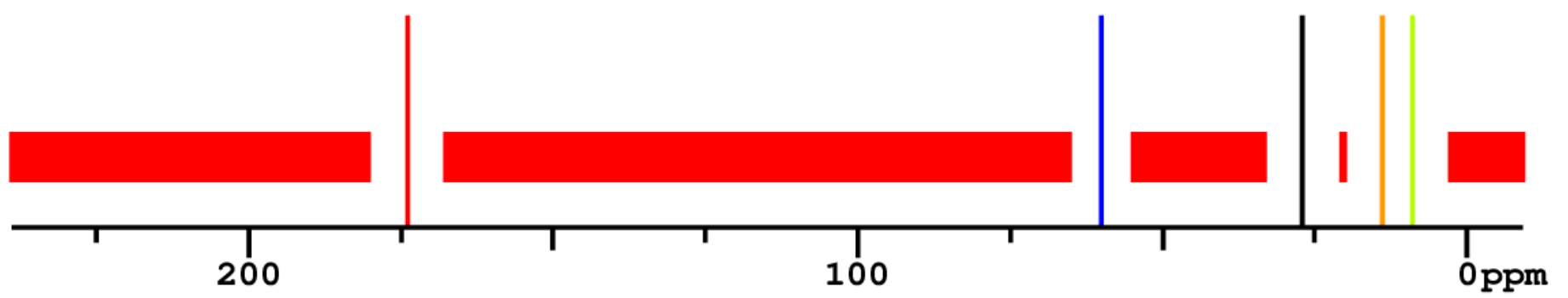
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

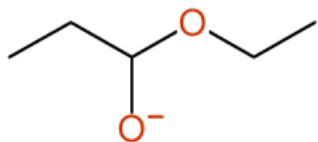
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[Back to Complete Result](#)

### Structure Proposal #3

Structure	Similarity Measure



Deviation = 3.31 ppm  
Similarity = 88 %

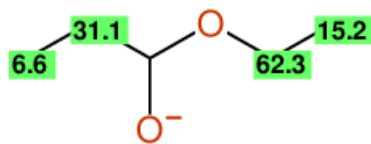
$C_5H_{11}O_2$

MWT = 103.06

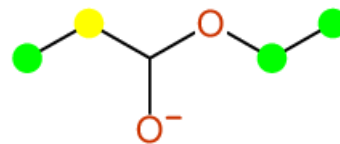
Search Web for this structure:

[GJYJNGCLZFAEMH](#)

Predicted Chemical Shiftvalues

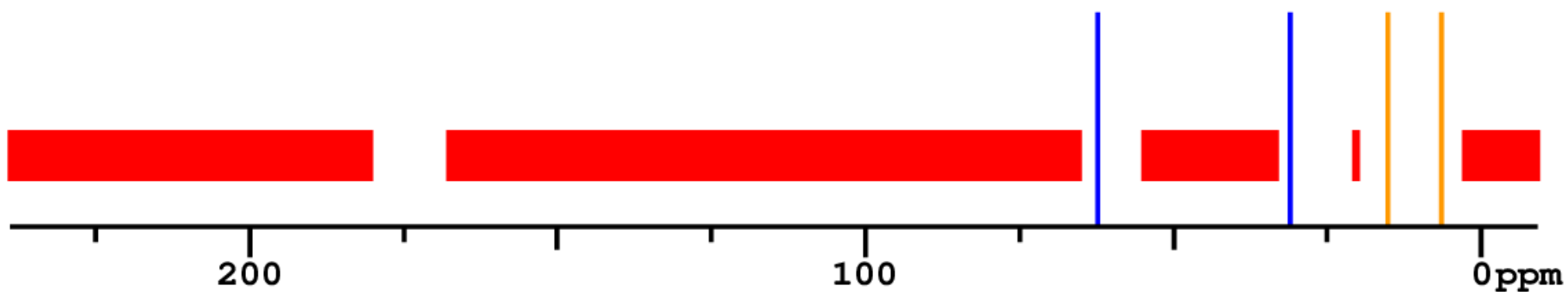


Matching Map




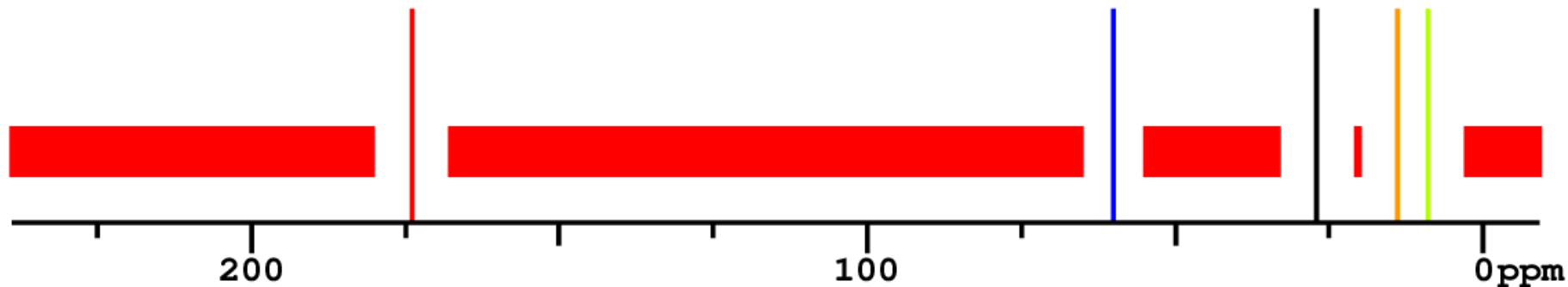
Predicted shift values

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



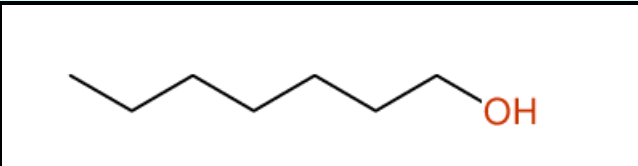
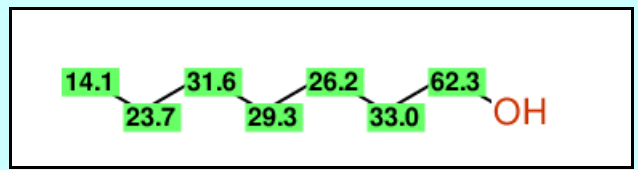

Experimental shift values

No line in reference: 



[Back to Complete Result](#)

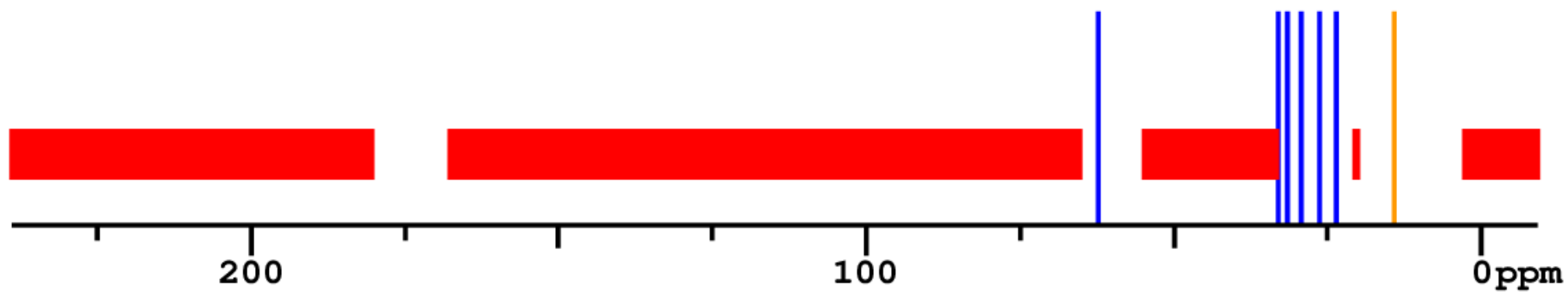
#### Structure Proposal #4

Structure	Similarity Measure
	<p>Deviation = 3.38 ppm Similarity = 71 % (Different pattern)</p> <p>C<sub>7</sub>O</p> <p>MWT = 100.08</p> <p>Search Web for this structure: <a href="#">ARYJKUMSSIOOH</a></p>
Predicted Chemical Shiftvalues	Matching Map
	



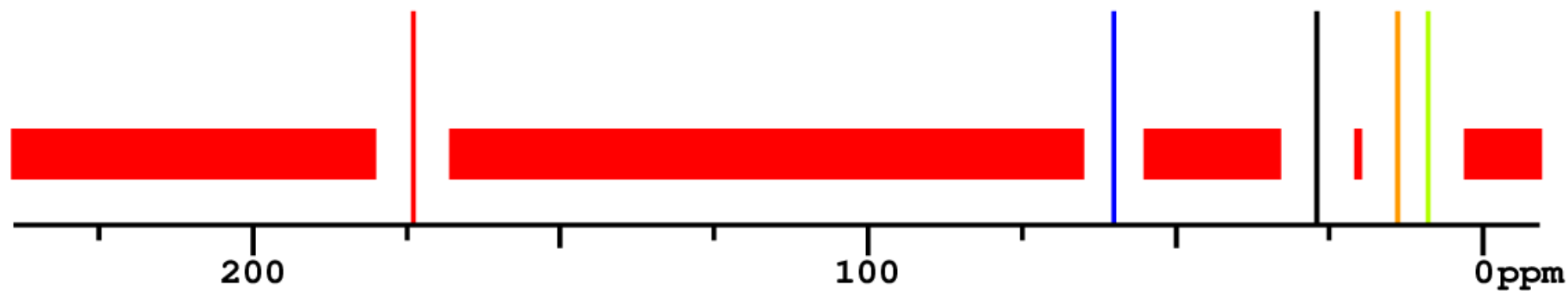
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

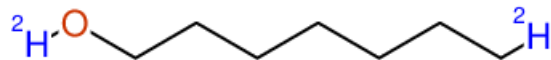
No line in reference: [red bar]



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### Structure Proposal #5

Structure	Similarity Measure



Deviation = 3.38 ppm  
 Similarity = 71 %  
 (Different pattern)



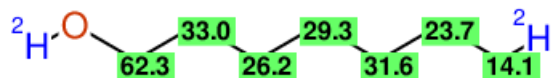
MWT = 118.08

Search Web for this structure:

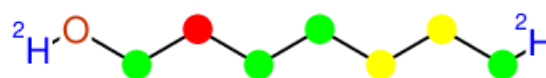
[BBMCTIGTTCKYKE](#)

[Availability](#)

Predicted Chemical Shiftvalues

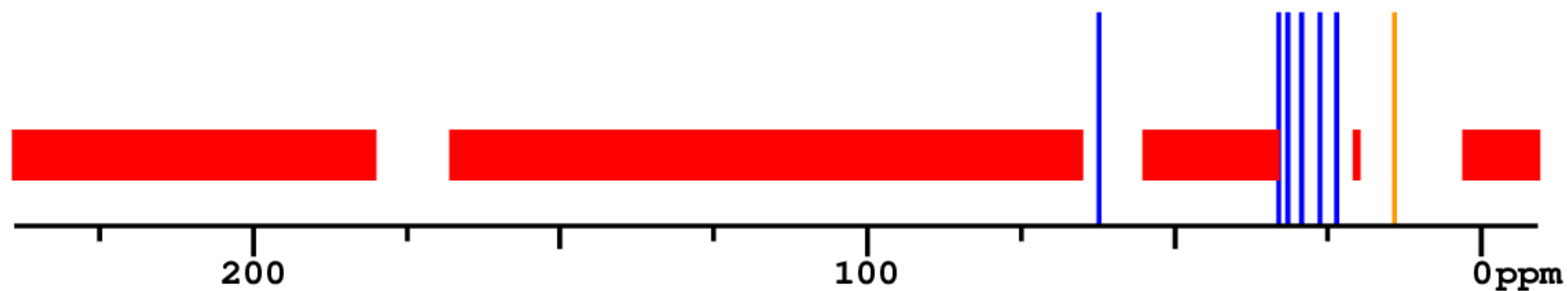


Matching Map



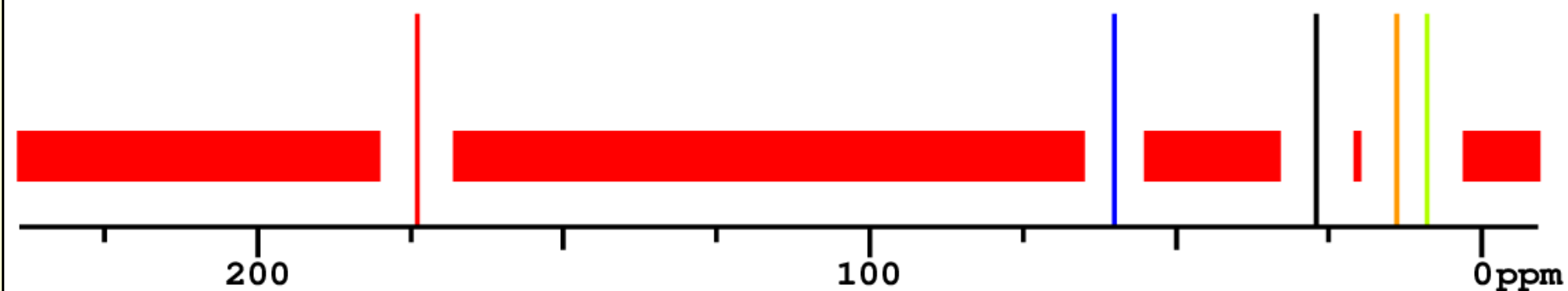
Predicted shift values

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



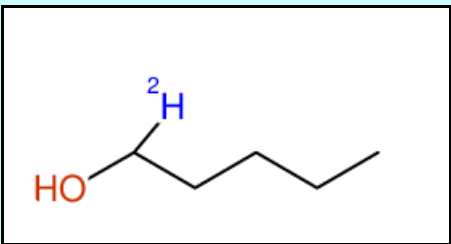
Experimental shift values

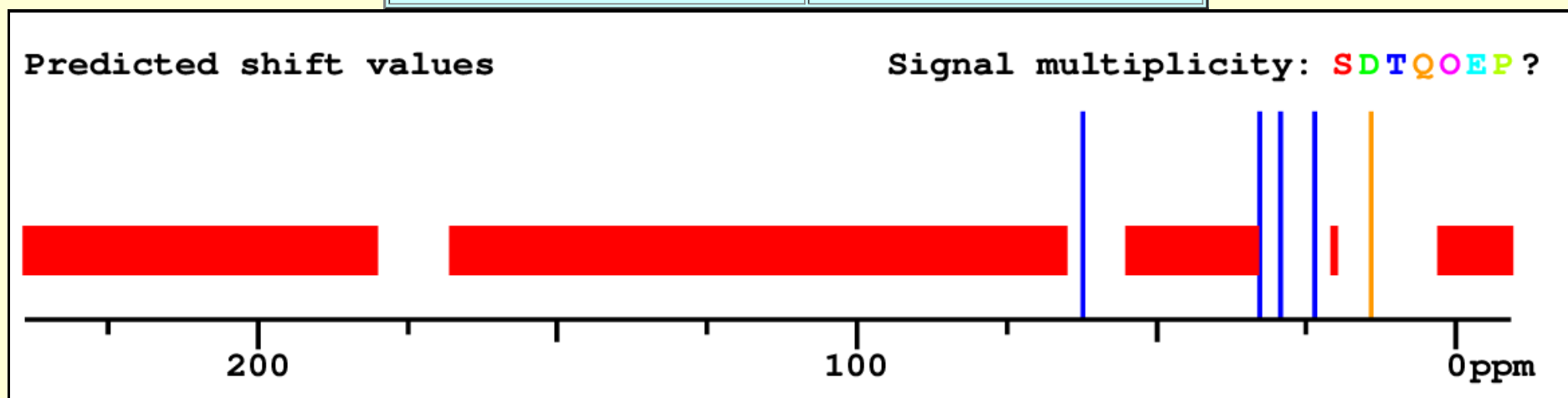
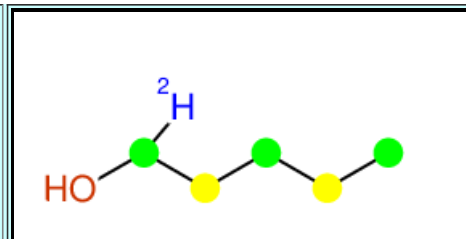
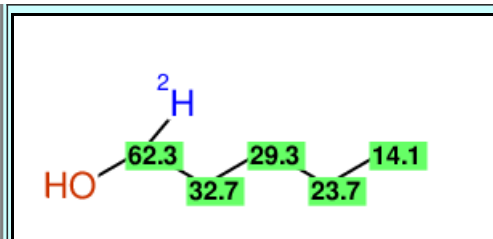
No line in reference:           




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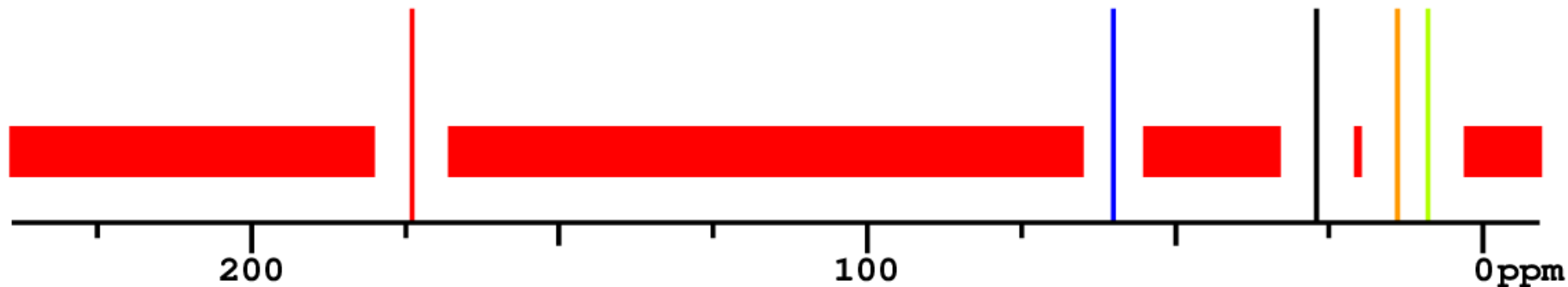
### Structure Proposal #6

Structure	Similarity Measure
	<p>Deviation = 3.40 ppm Similarity = 80 %</p> <p><math>C_5H_{12}O</math></p> <p>MWT = 89.06</p> <p>Search Web for this structure: <a href="#">AMQJEAYHLZJPGS</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



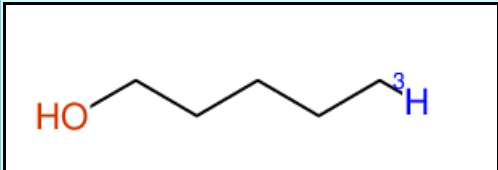
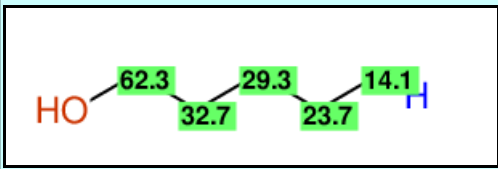
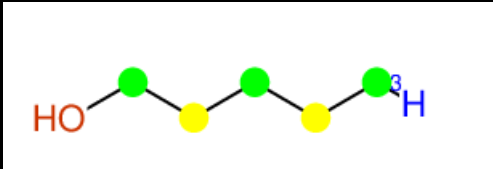
Experimental shift values

No line in reference: 



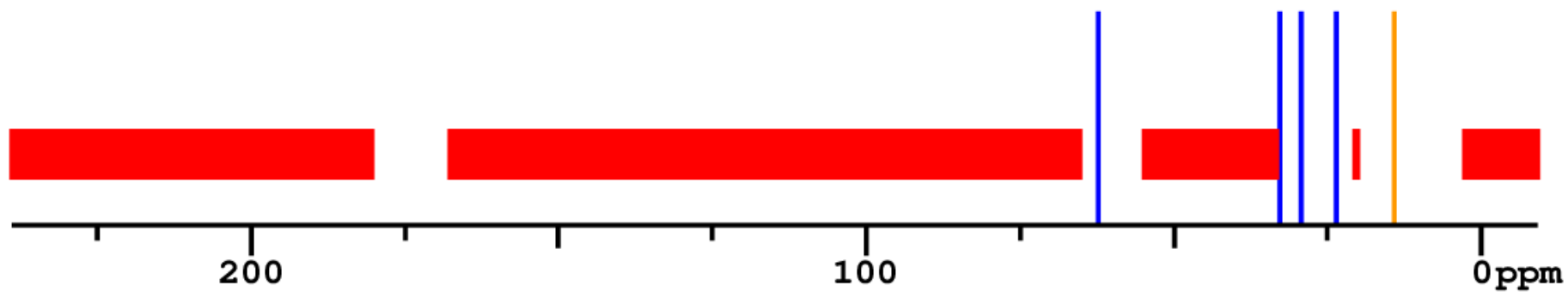
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### Structure Proposal #7

Structure	Similarity Measure
	Deviation = 3.40 ppm Similarity = 80 %  C <sub>5</sub> H <sub>12</sub> O  MWT = 90.06  Search Web for this structure:  <a href="#">AMQJEAYHLZJPGS</a>  <a href="#">Availability</a>
Predicted Chemical Shiftvalues	Matching Map
	

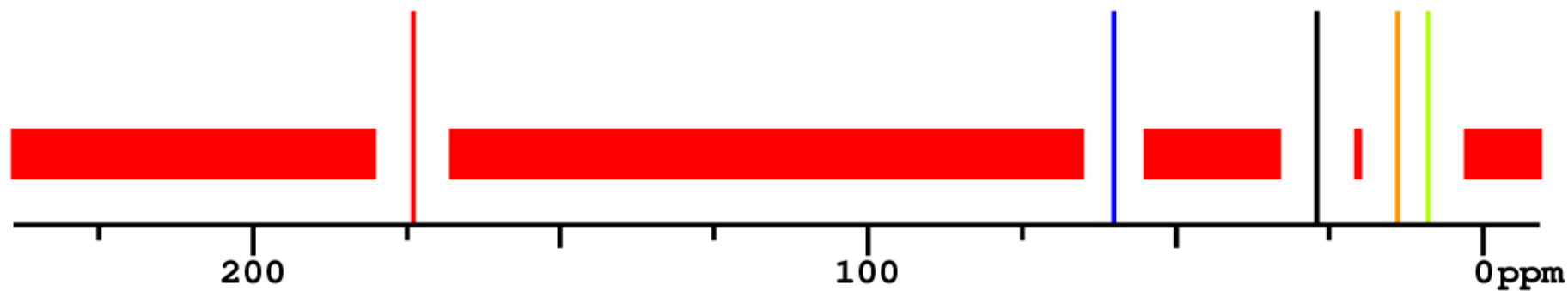
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

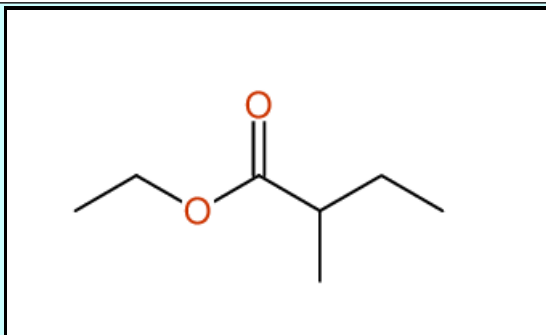
No line in reference: [red bar]



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### Structure Proposal #8

Structure	Similarity Measure



Deviation = 3.41 ppm  
Similarity = 86 %  
(Different pattern)

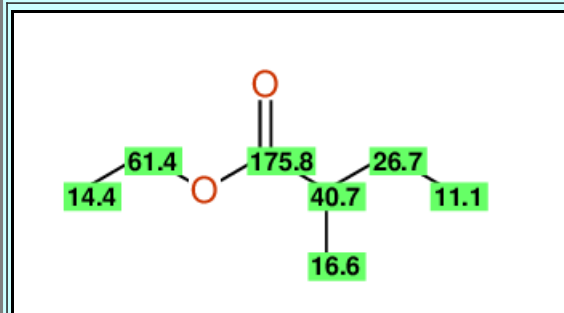
$C_7O_2$

MWT = 116.08

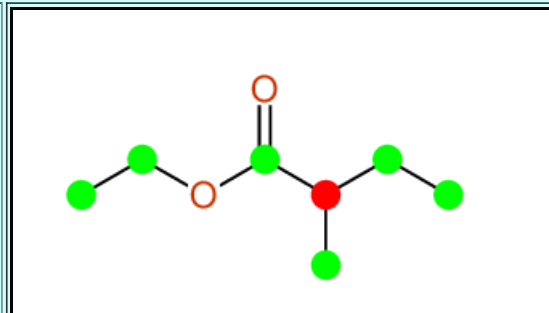
Search Web for this structure:

[JPVJJBICKBKSH](#)

### Predicted Chemical Shiftvalues

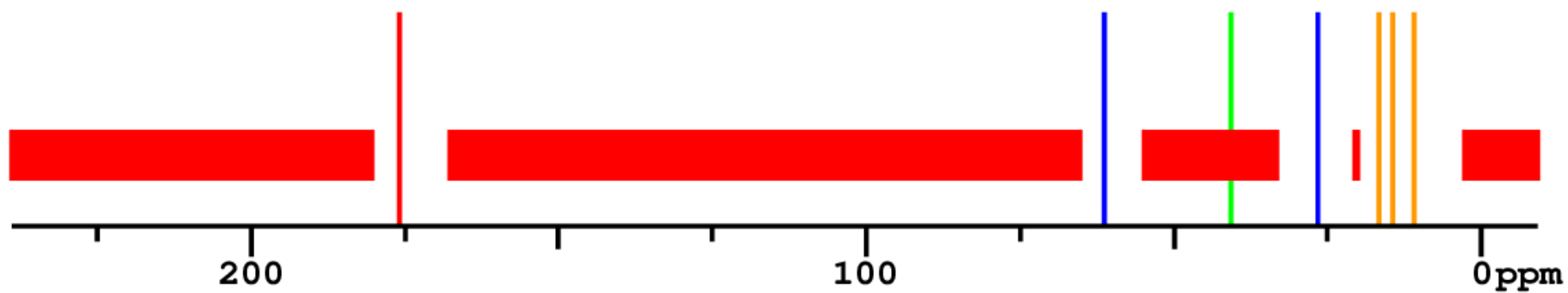


### Matching Map



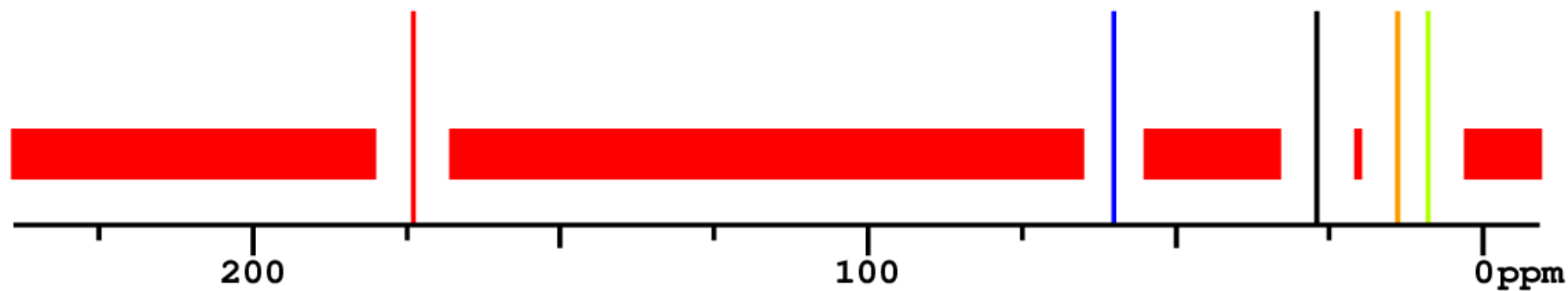
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

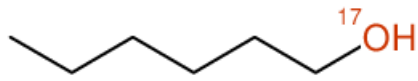


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### Structure Proposal #9

Structure	Similarity Measure





Deviation = 3.44 ppm  
Similarity = 67 %  
(Different pattern)

$C_6H_{14}O$

MWT = 103.07

Search Web for this structure:

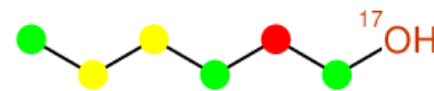
[ZSIAUFGUXNUGDI](#)

[Availability](#)

Predicted Chemical Shiftvalues

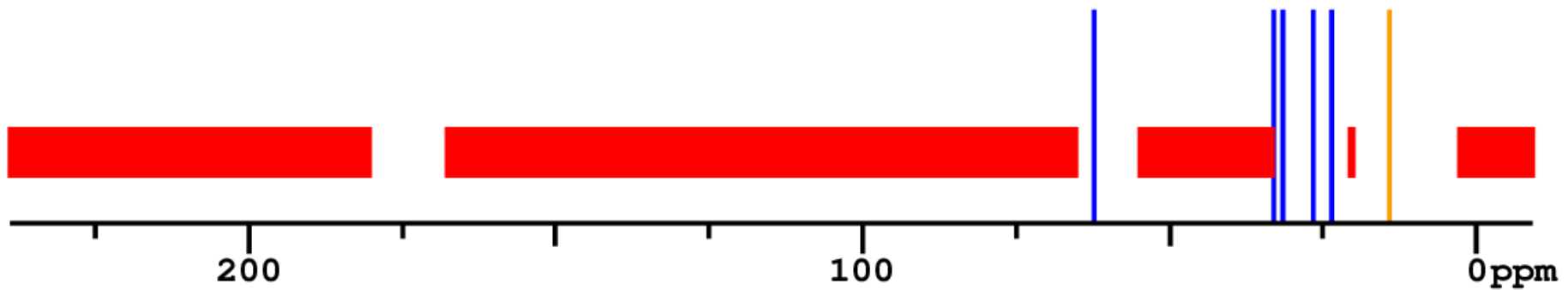


Matching Map



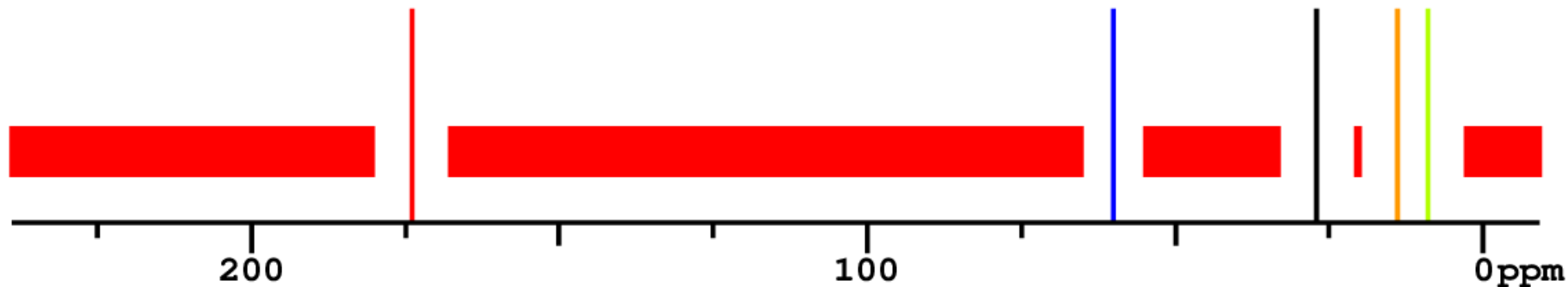
Predicted shift values

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



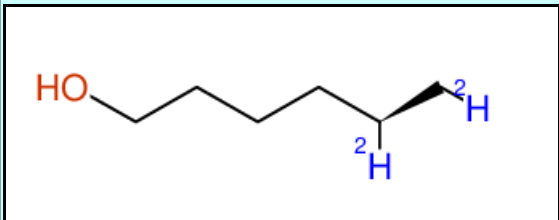
Experimental shift values

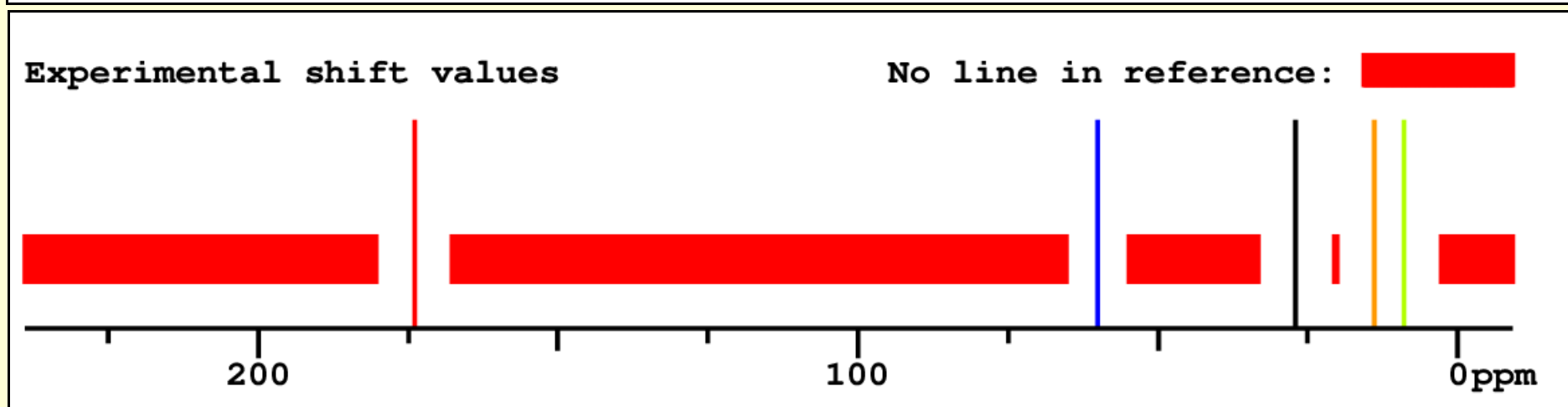
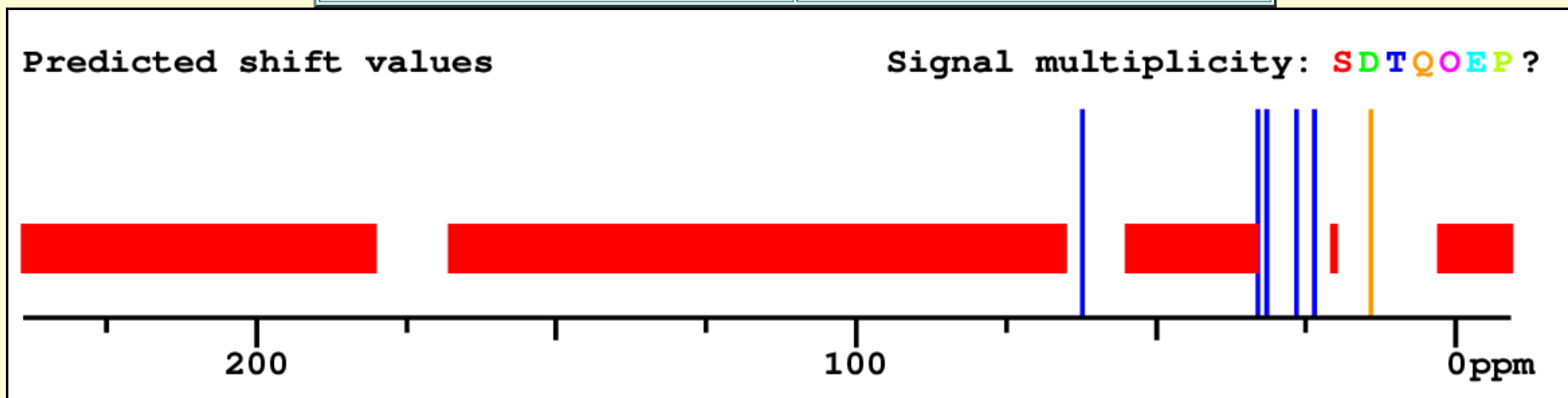
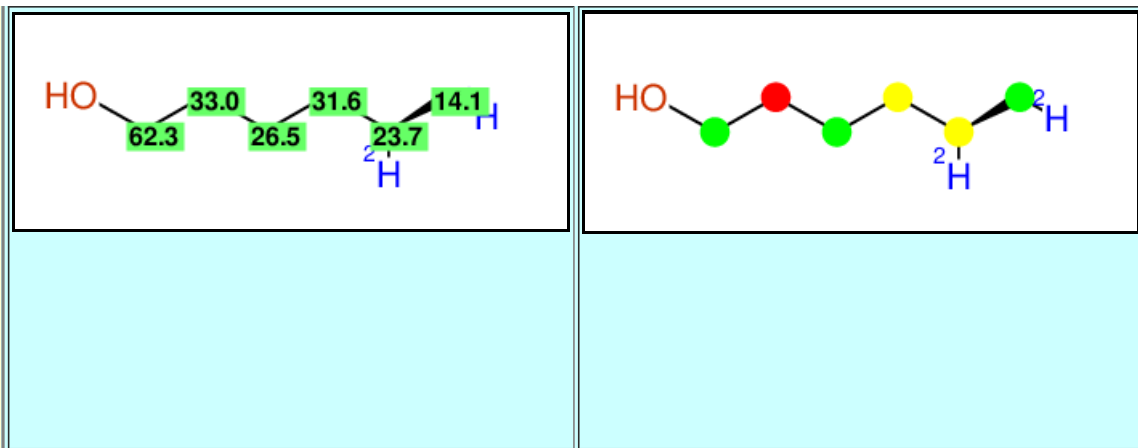
No line in reference: 



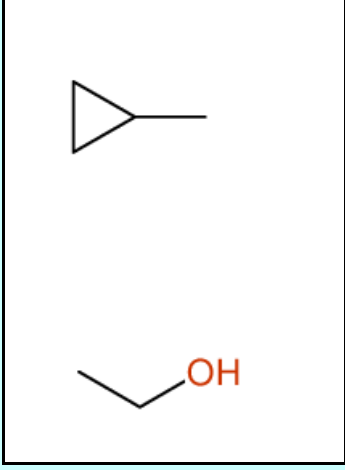
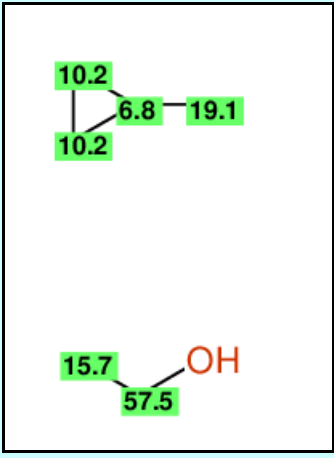
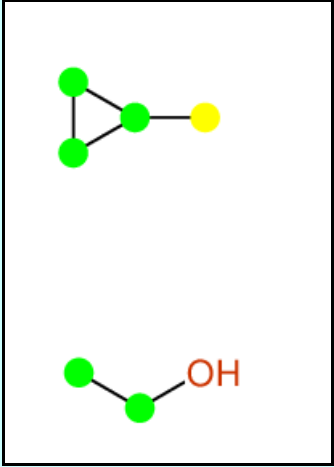
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### Structure Proposal #10

Structure	Similarity Measure
 <p>Chemical structure of 1-hexanol (<math>C_6H_{14}O</math>) is shown. The structure is a six-carbon chain with a hydroxyl group (HO) at the end. Two protons are labeled with a blue '2' and 'H', indicating their chemical environment.</p>	<p>Deviation = 3.44 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{14}O</math></p> <p>MWT = 104.07</p> <p>Search Web for this structure: <a href="#">ZSIAUFGUXNUGDI</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map

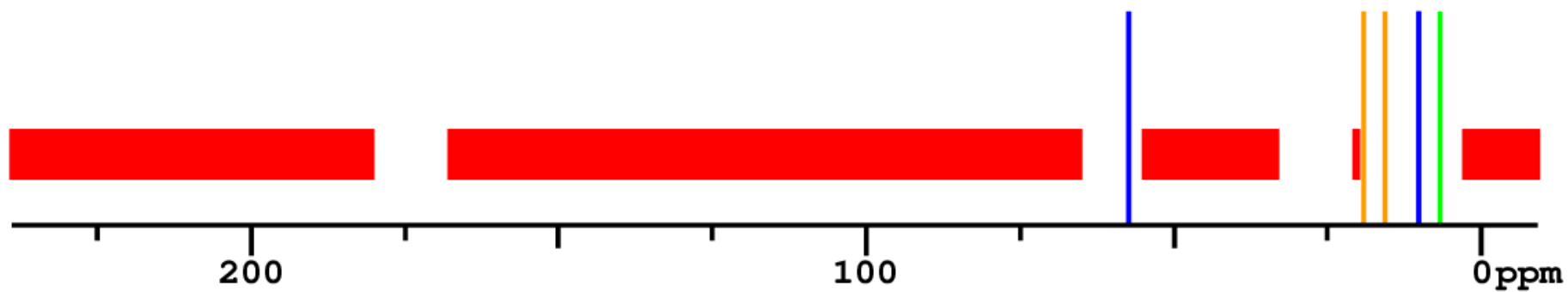


### Structure Proposal #11

Structure	Similarity Measure
 <p>The top structure is cyclopropanol, a three-membered carbon ring with a hydroxyl group. The bottom structure is ethanol, a two-carbon chain with a hydroxyl group.</p>	<p>Deviation = 3.56 ppm Similarity = 92 %</p> <p><math>C_4H_8 \cdot C_2H_6O</math></p> <p>MWT = 102.07</p> <p>Search Web for this structure: <a href="#">OTVBAIYRCXJKL</a></p>
Predicted Chemical Shiftvalues	Matching Map
 <p>The top structure (cyclopropanol) has predicted chemical shift values of 10.2 ppm for the ring carbons and 6.8 ppm for the hydroxyl carbon. The bottom structure (ethanol) has predicted chemical shift values of 15.7 ppm for the methyl carbon and 57.5 ppm for the methylene carbon.</p>	 <p>The matching map shows the correspondence between atoms in the two structures. The top structure has four green dots representing carbons and one yellow dot representing the oxygen. The bottom structure has three green dots representing carbons and one yellow dot representing the oxygen. Lines connect the dots to show the mapping between the two structures.</p>

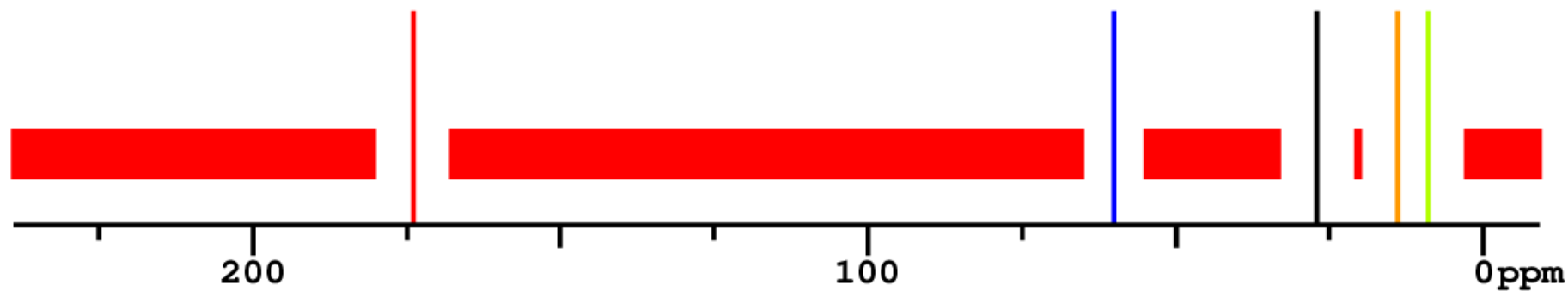
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

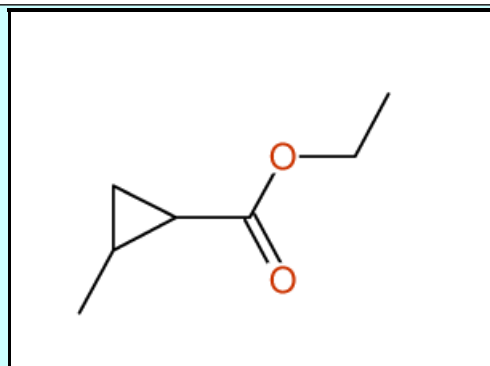
No line in reference: [red bar]



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### Structure Proposal #12

Structure	Similarity Measure



Deviation = 3.72 ppm  
Similarity = 64 %

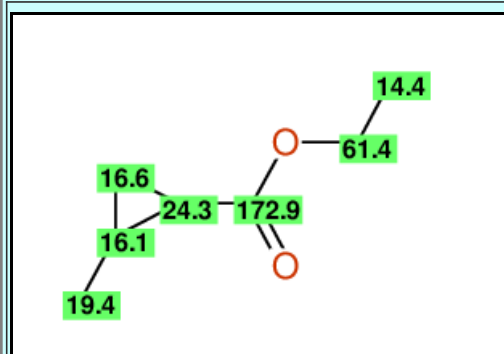
$C_7O_2$

MWT = 116.08

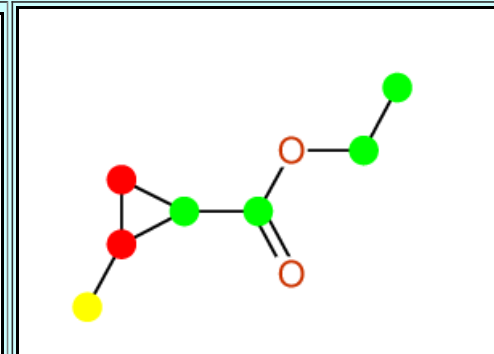
Search Web for this structure:

[ZNXRPIKPYJZPNI](#)

### Predicted Chemical Shiftvalues

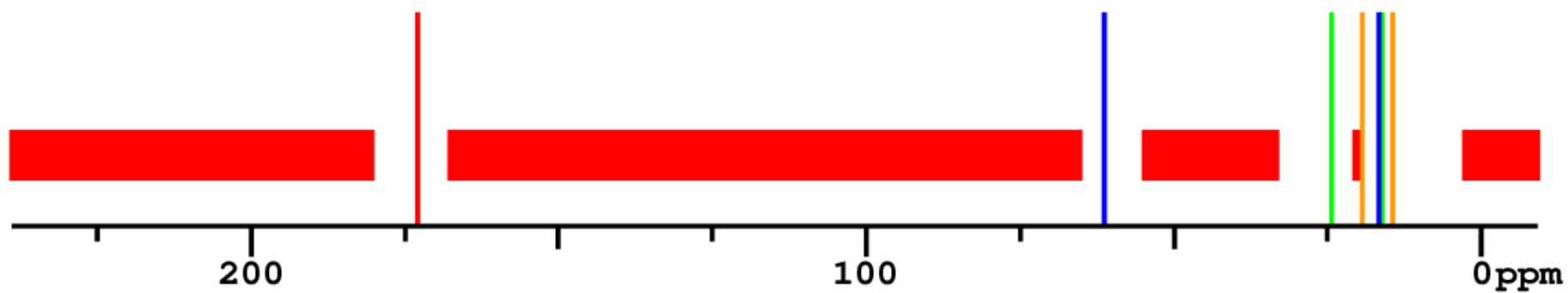


### Matching Map



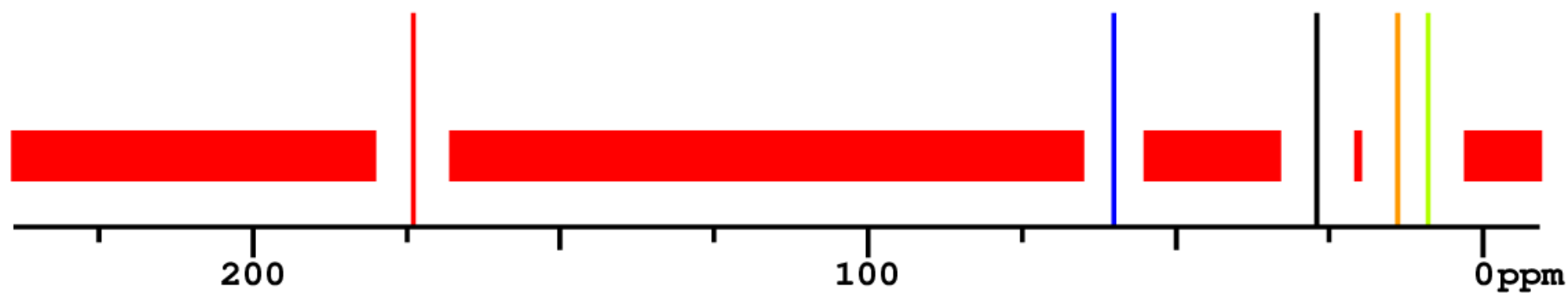
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

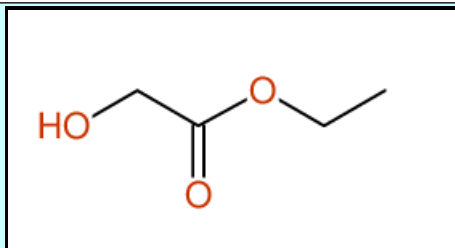
No line in reference: [red bar]



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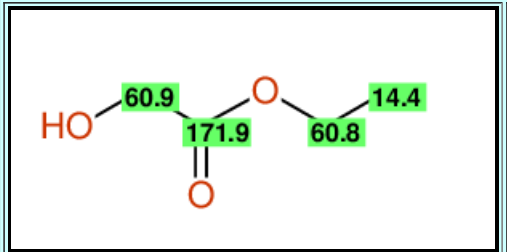
### Structure Proposal #13

Structure	Similarity Measure

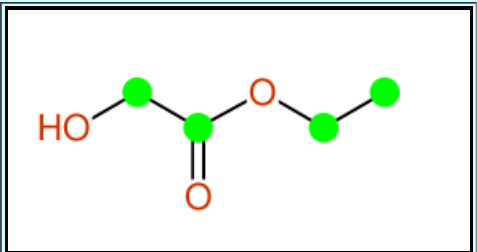


Deviation = 3.72 ppm  
Similarity = 100 %  
  
 $C_4O_3$   
  
MWT = 96.04  
  
Search Web for this structure:  
[USTOPXSKJLOMKG](#)

Predicted Chemical Shiftvalues

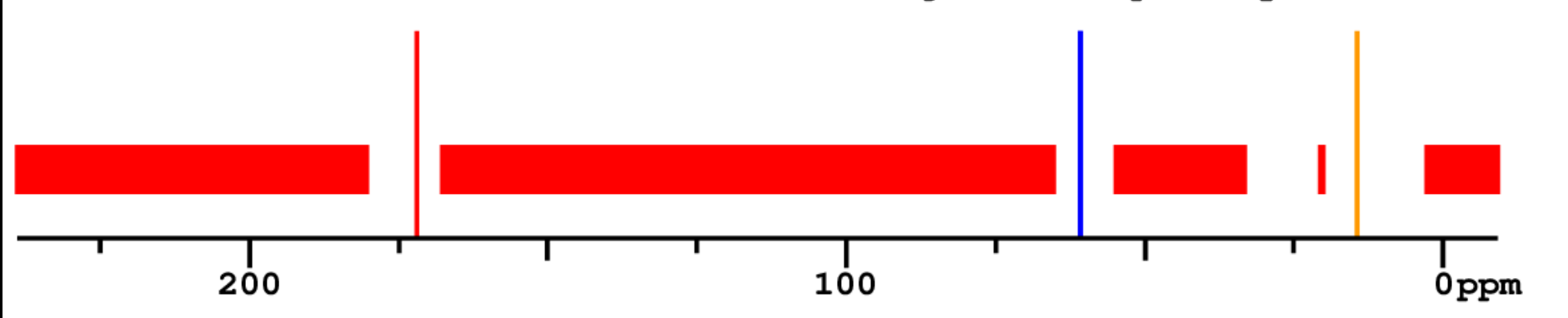


Matching Map



Predicted shift values

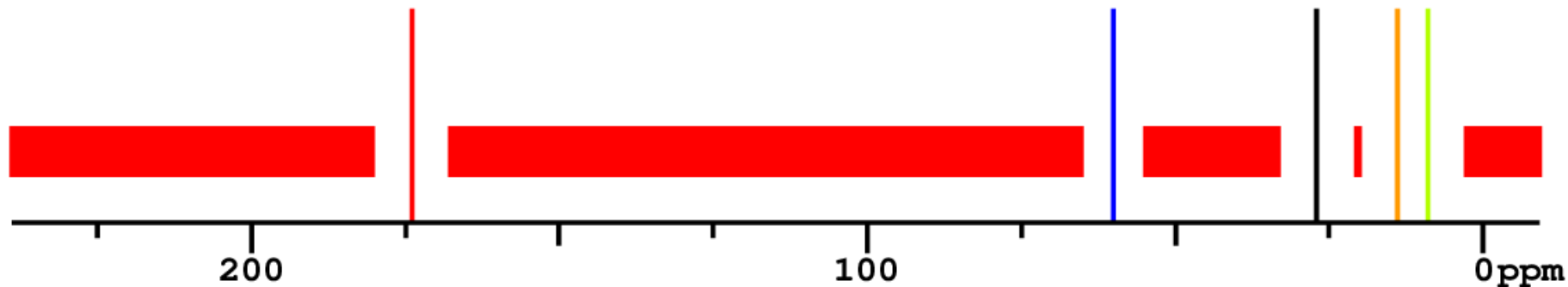
Signal multiplicity: **S****D****T****Q****O****E****P**?





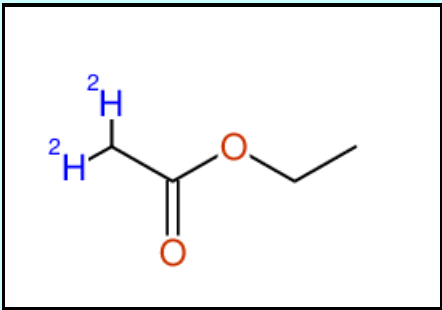
Experimental shift values

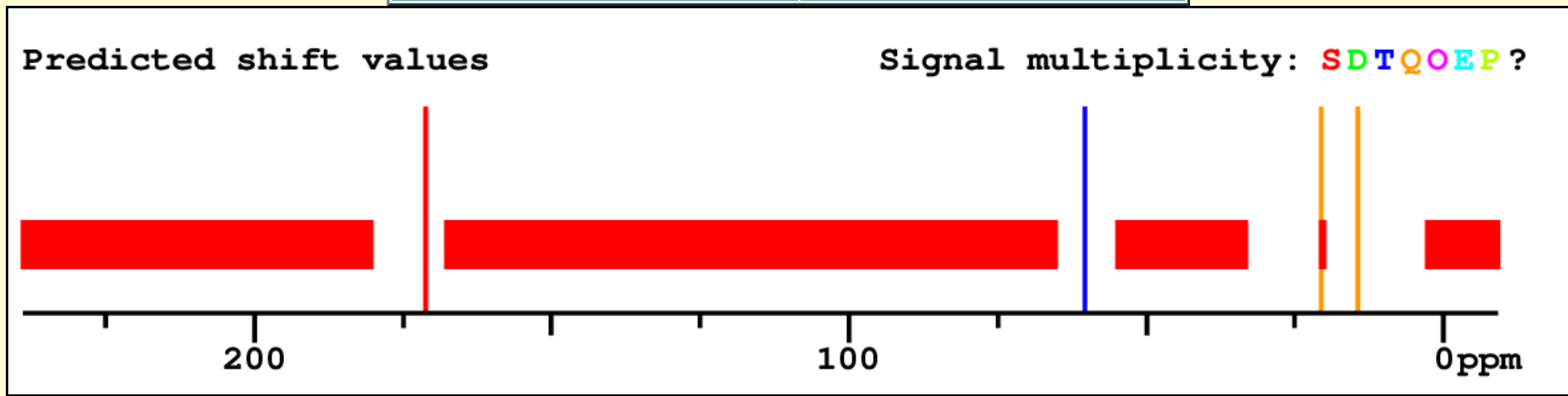
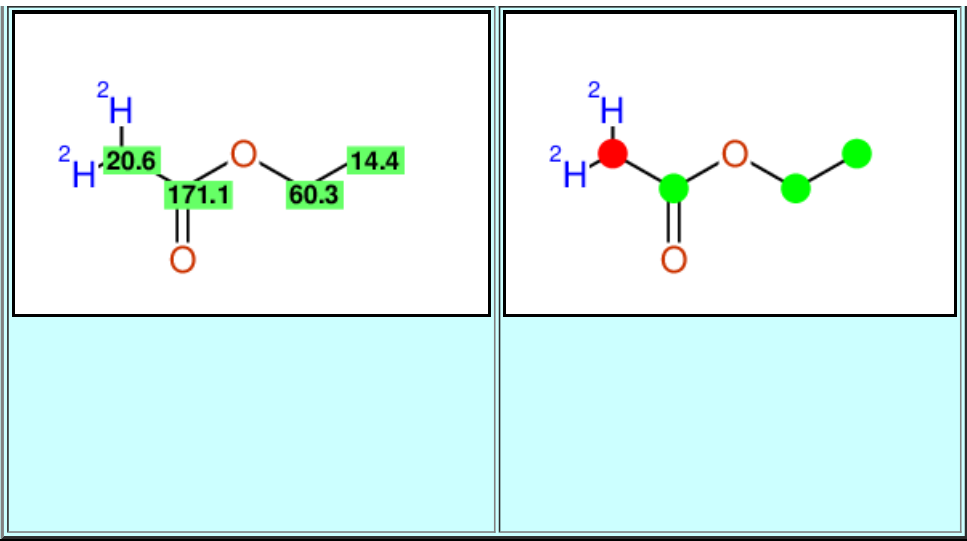
No line in reference: ██████████



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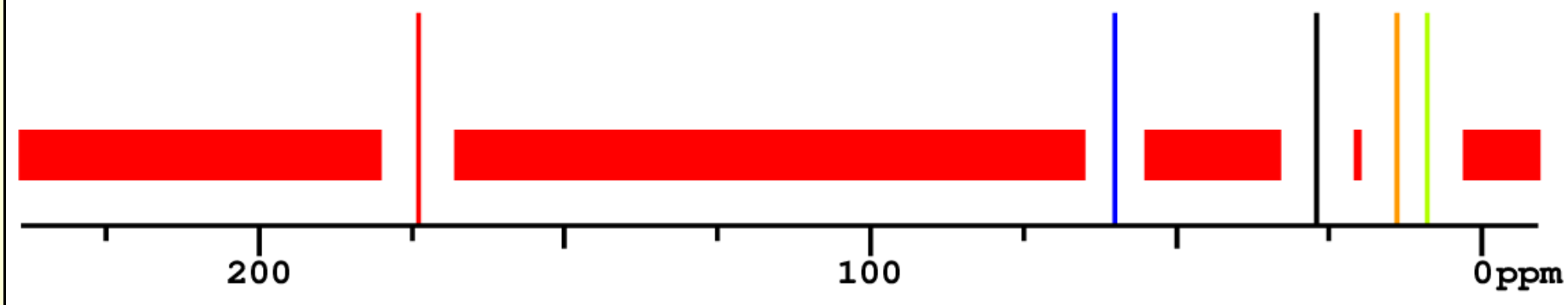
### Structure Proposal #14

Structure	Similarity Measure
	<p>Deviation = 3.74 ppm Similarity = 75 % (Different pattern)</p> <p><math>C_4H_8O_2</math></p> <p>MWT = 90.04</p> <p>Search Web for this structure: <a href="#">XEKOWRVHYACXQJ</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



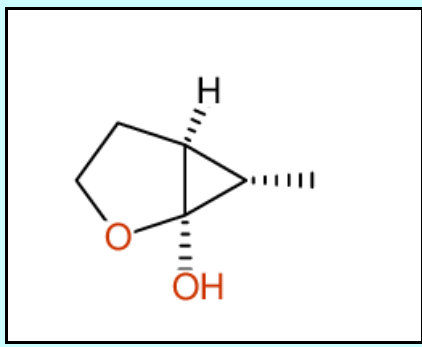
Experimental shift values

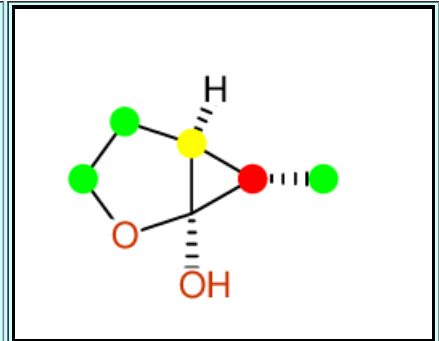
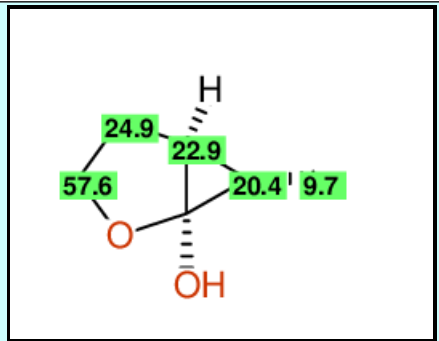
No line in reference: 



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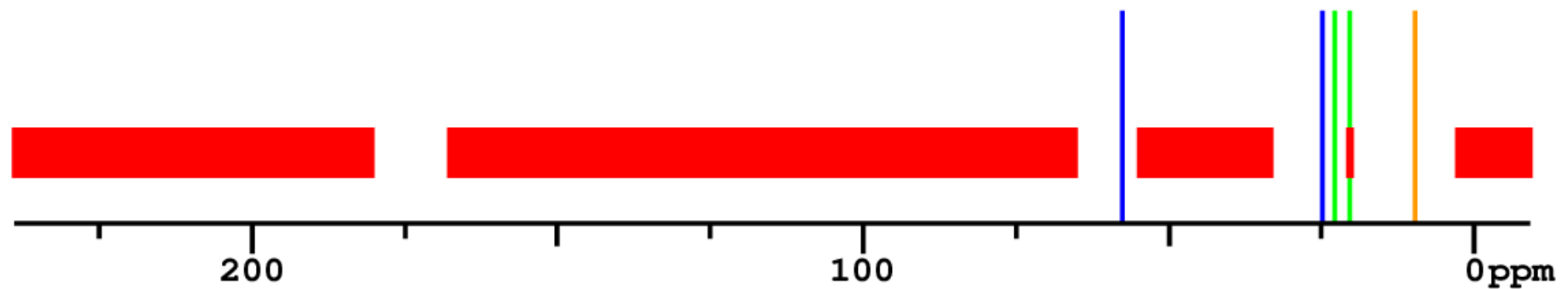
### Structure Proposal #15

Structure	Similarity Measure
	<p>Deviation = 3.77 ppm Similarity = 70 % (Different pattern)</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.07</p> <p>Search Web for this structure: <a href="#">OKQNTQARVDVCHK</a></p>
Predicted Chemical Shiftvalues	Matching Map



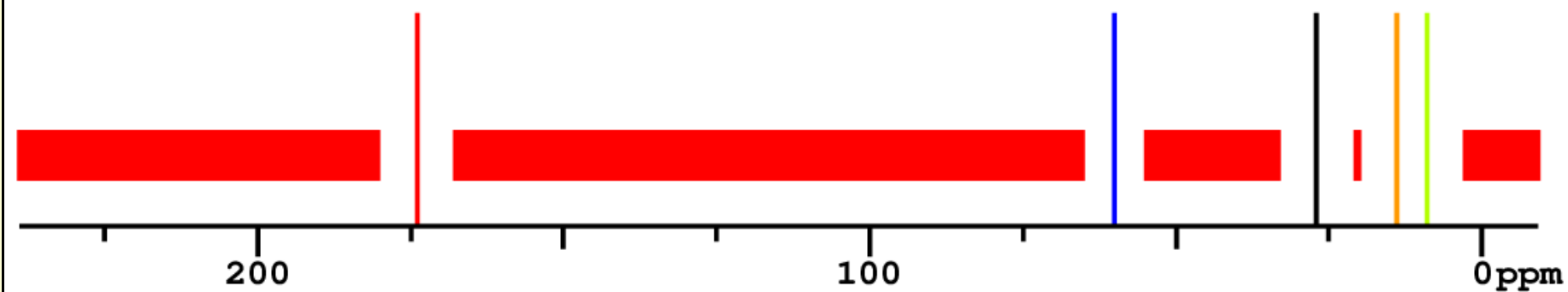
Predicted shift values

Signal multiplicity: S D T Q O E P ?



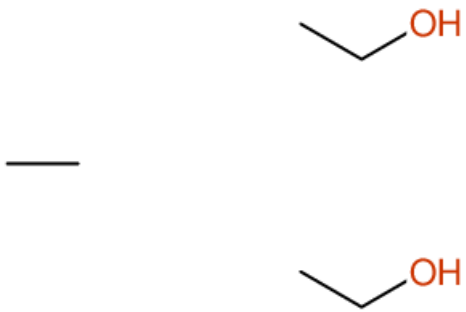
Experimental shift values

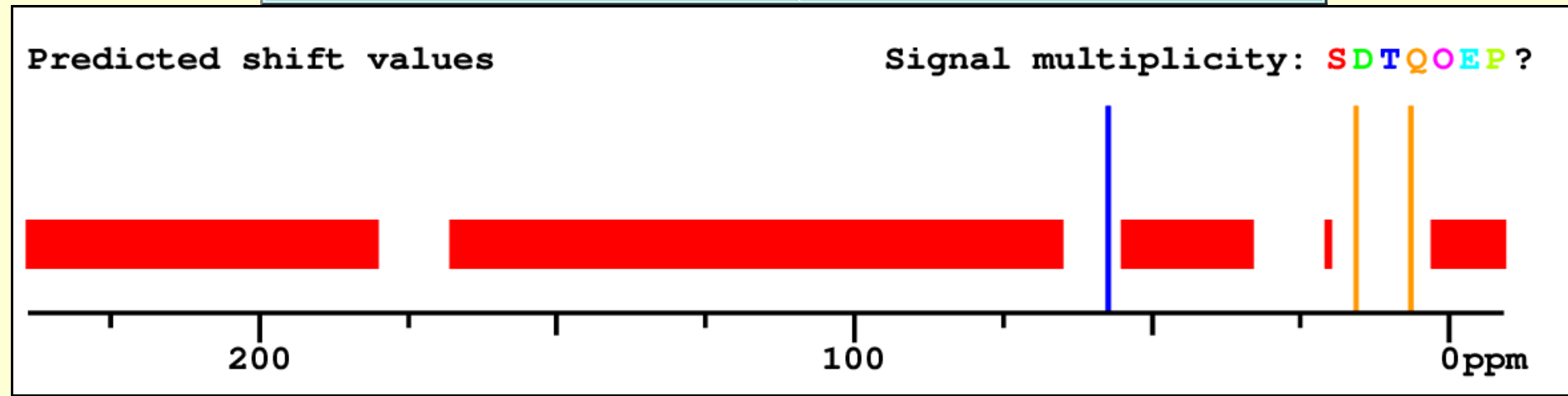
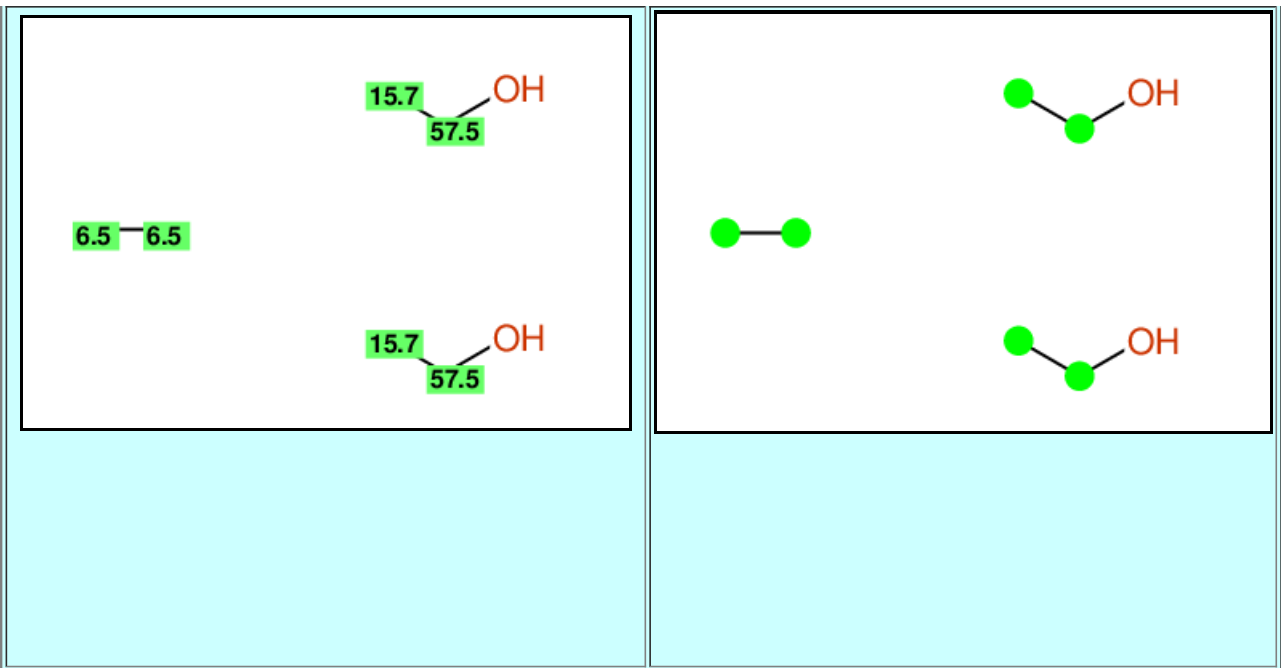
No line in reference: 



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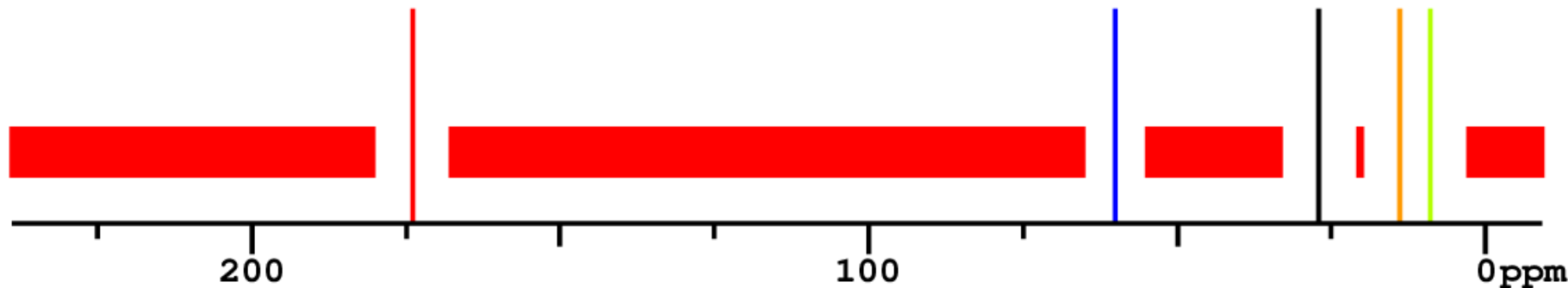
### Structure Proposal #16

Structure	Similarity Measure
 <p>The structure shows a skeletal structure of ethanol (CH<sub>3</sub>CH<sub>2</sub>OH) with the hydroxyl group (OH) highlighted in red. A horizontal line is drawn below the structure.</p>	<p>Deviation = 4.04 ppm Similarity = 100 %</p> <p><chem>2C2H6O.C2H6</chem></p> <p>MWT = 116.07</p> <p>Search Web for this structure: <a href="#">MKNBWAXUAMKIOZ</a></p>
<b>Predicted Chemical Shiftvalues</b>	<b>Matching Map</b>



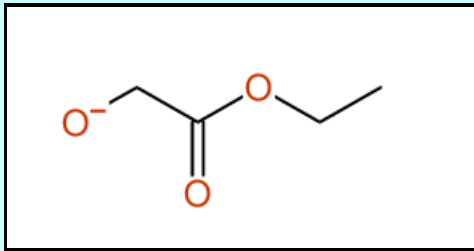
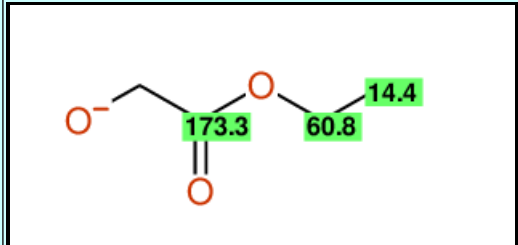
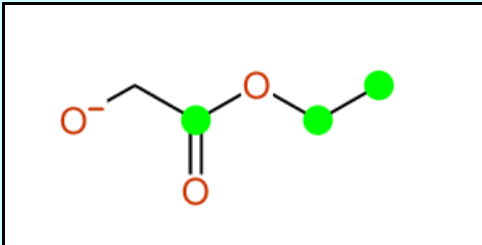
Experimental shift values

No line in reference: 



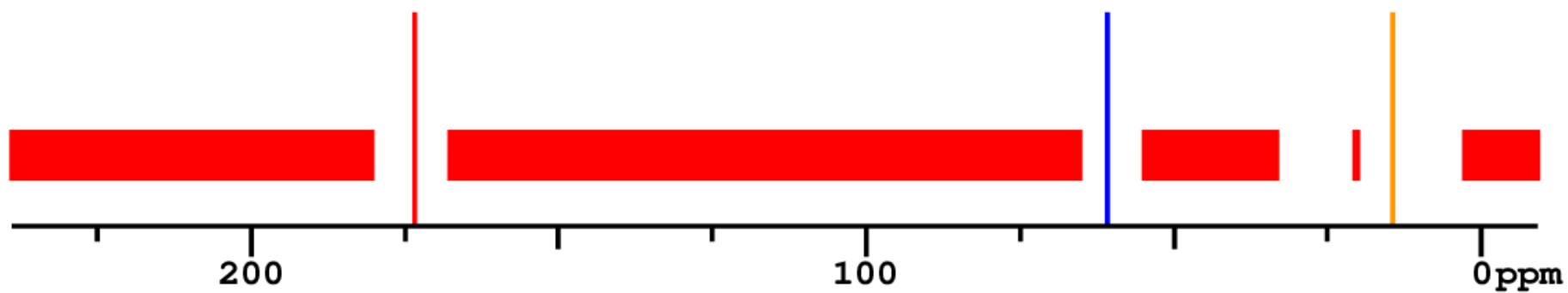
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### Structure Proposal #17

Structure	Similarity Measure
	Deviation = 4.11 ppm Similarity = 100 %  C <sub>4</sub> H <sub>7</sub> O <sub>3</sub>  MWT = 103.04  Search Web for this structure:  <a href="#">PDHCCQJYEKLVRY</a>
Predicted Chemical Shiftvalues	Matching Map
	

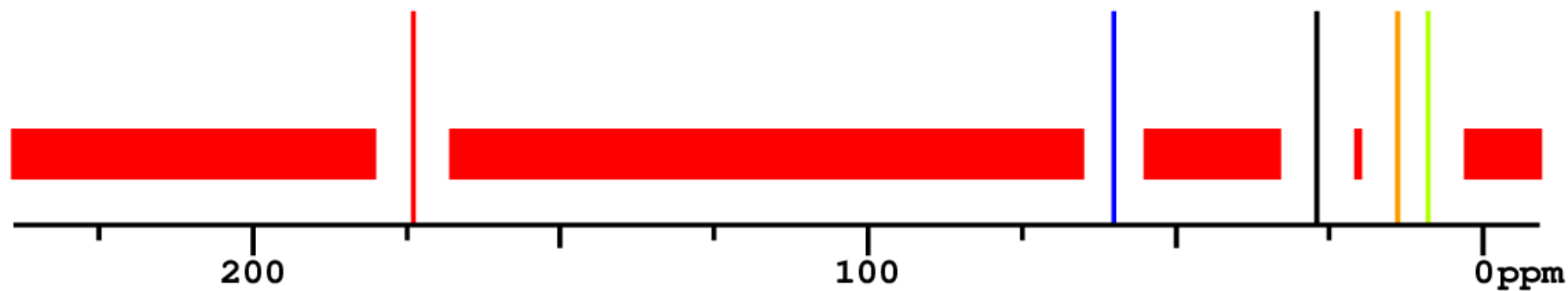
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

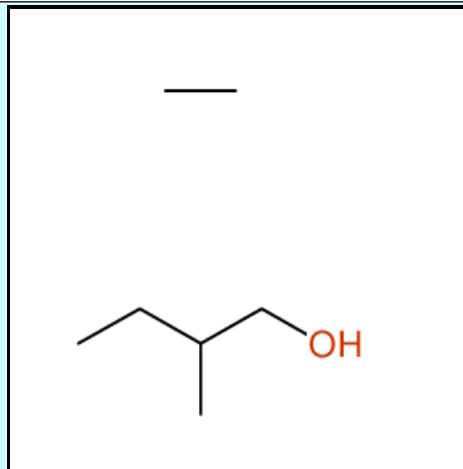


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### Structure Proposal #18

Structure	Similarity Measure





Deviation = 4.15 ppm  
Similarity = 71 %  
(Different pattern)



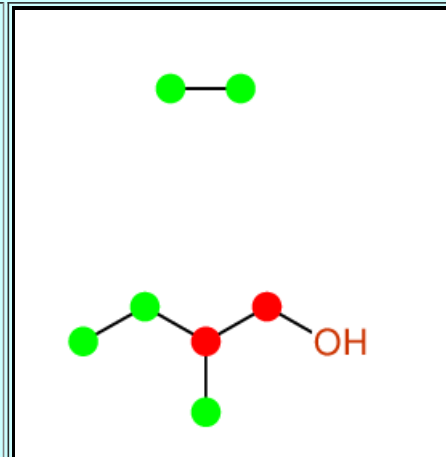
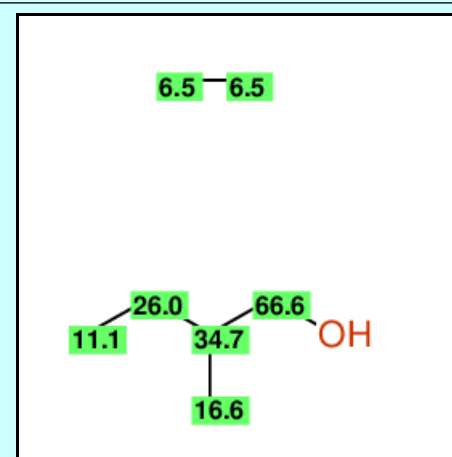
MWT = 118.08

Search Web for this structure:

[QSLNWESTNWAUCD](#)

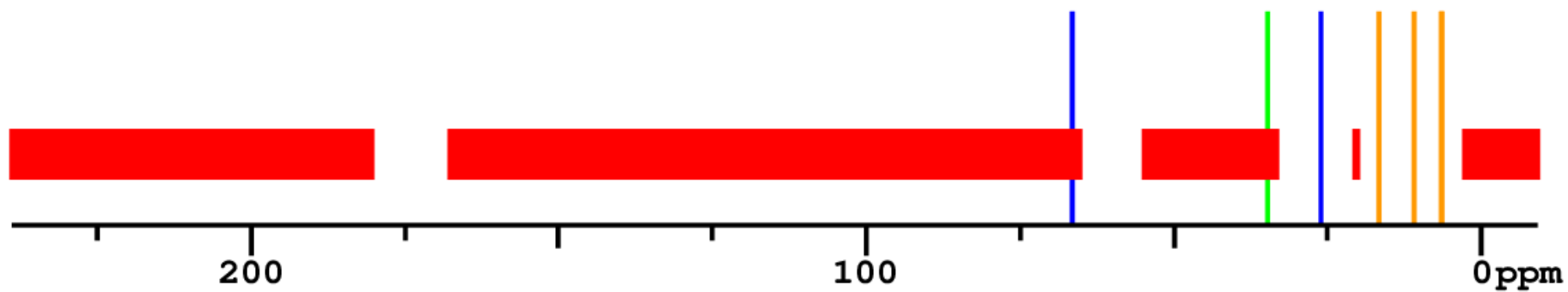
Predicted Chemical  
Shiftvalues

Matching Map



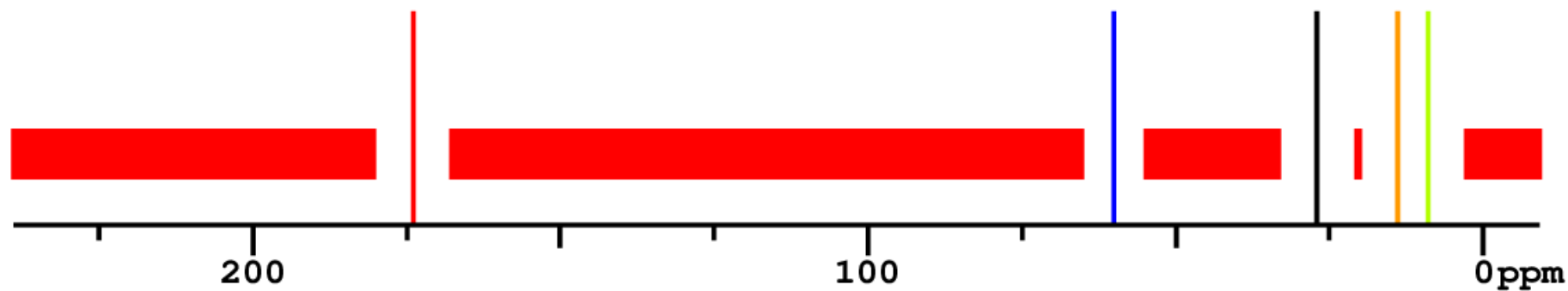
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

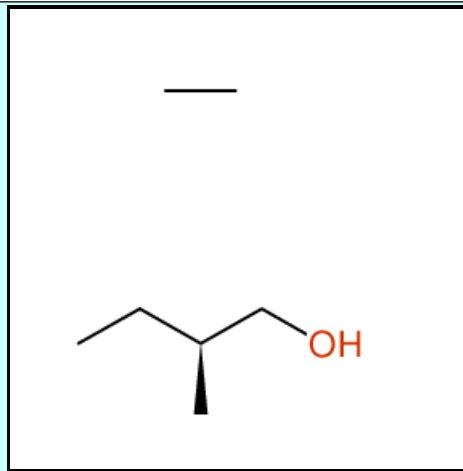
No line in reference: [red bar]



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### Structure Proposal #19

Structure	Similarity Measure



Deviation = 4.15 ppm  
Similarity = 71 %  
(Different pattern)



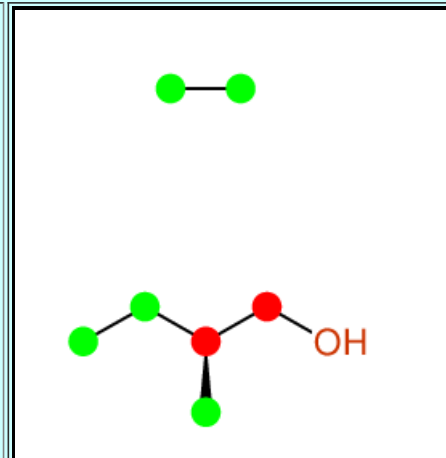
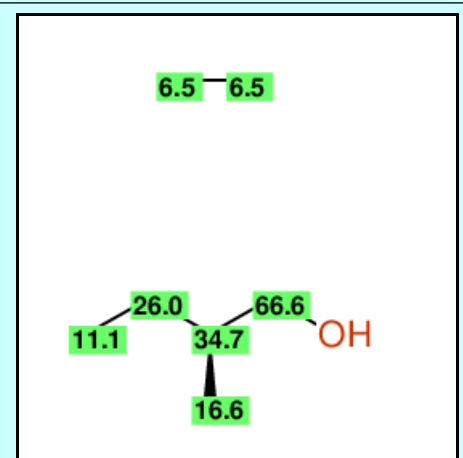
MWT = 118.08

Search Web for this structure:

[QSLNWESTNWAUCD](#)

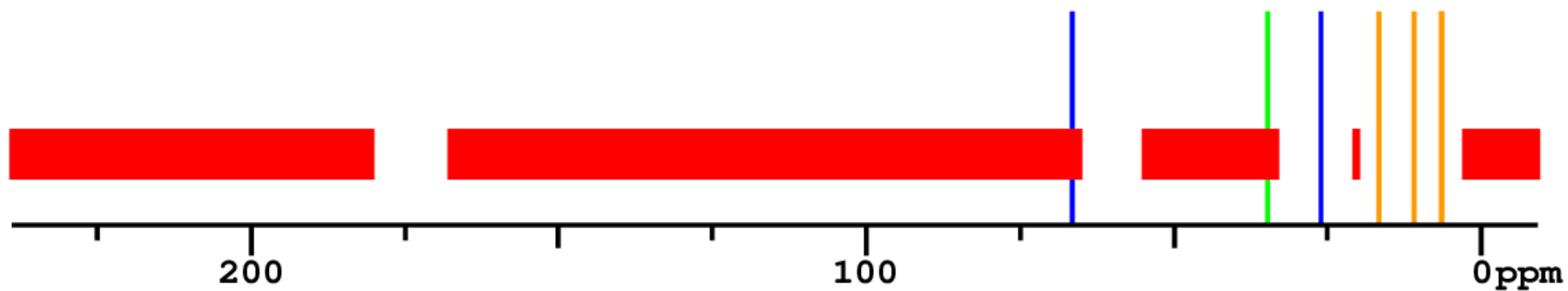
Predicted Chemical  
Shiftvalues

Matching Map



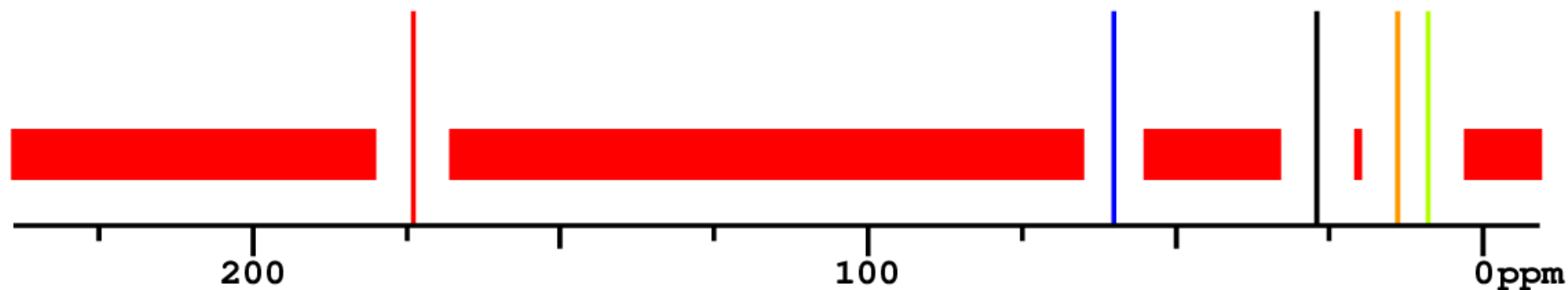
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

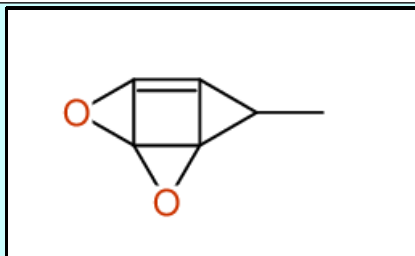
No line in reference: [red bar]



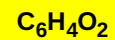
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### Structure Proposal #20

Structure	Similarity Measure



Deviation = 4.26 ppm  
Similarity = 100 %



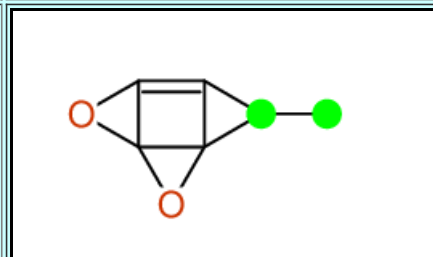
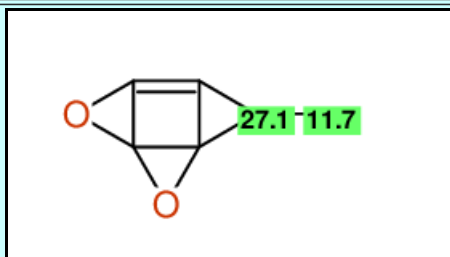
MWT = 108.07

Search Web for this structure:

[HFYMLXNNBCFAY](#)

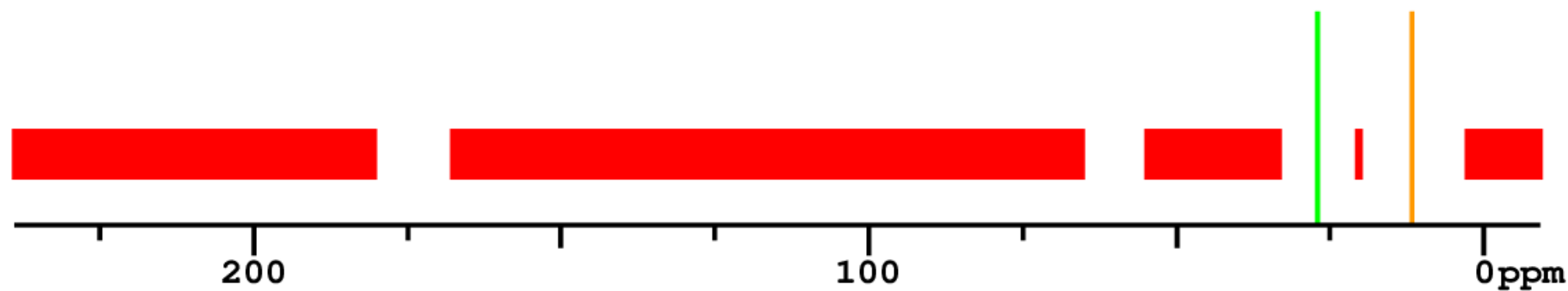
Predicted Chemical Shiftvalues

Matching Map




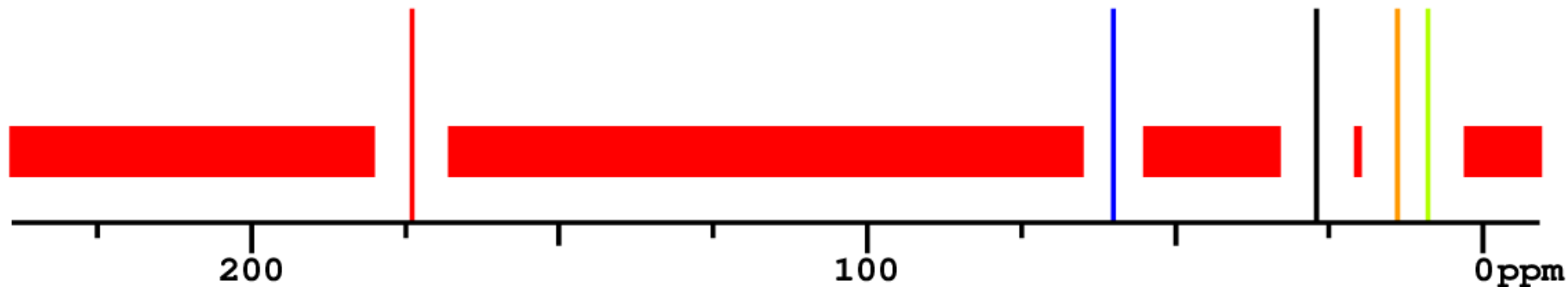
Predicted shift values

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



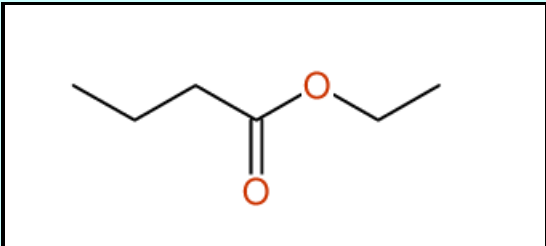
Experimental shift values

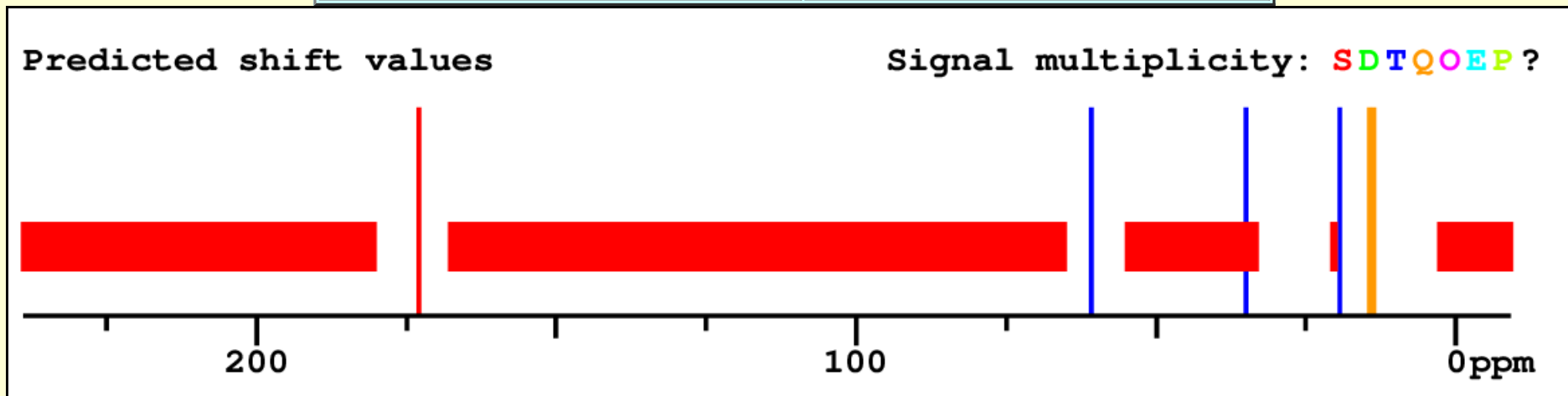
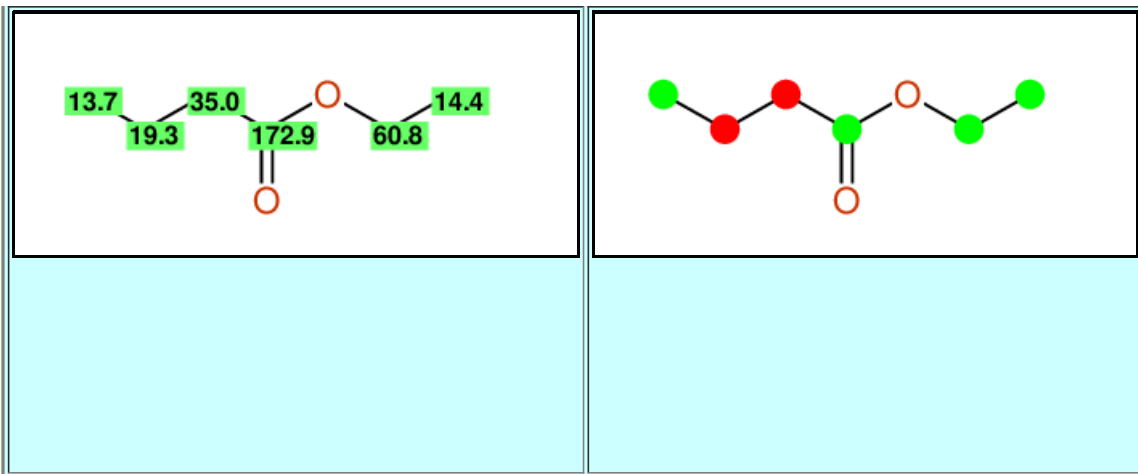
No line in reference: 




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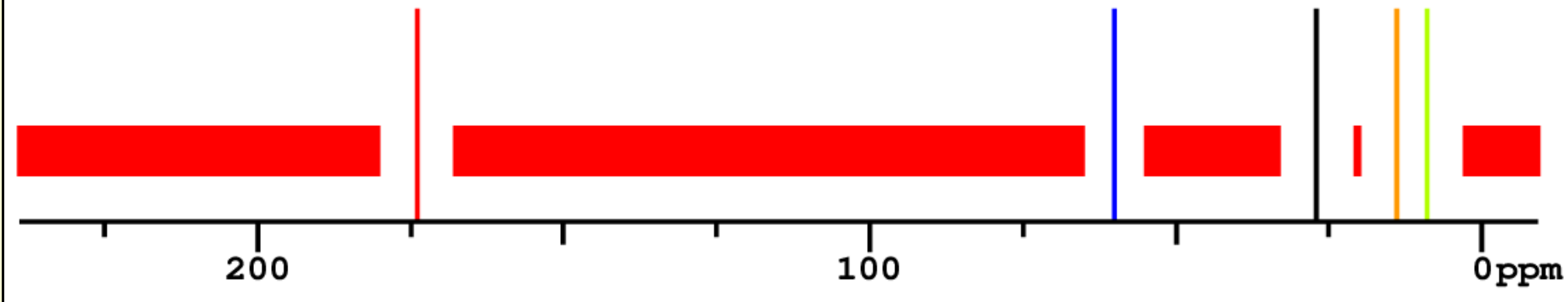
### Structure Proposal #21

Structure	Similarity Measure
	<p>Deviation = 4.32 ppm Similarity = 67 % (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="#">OBNCKNCVKJNDBV</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



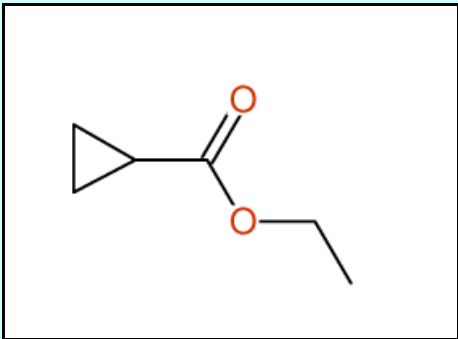
Experimental shift values

No line in reference: 

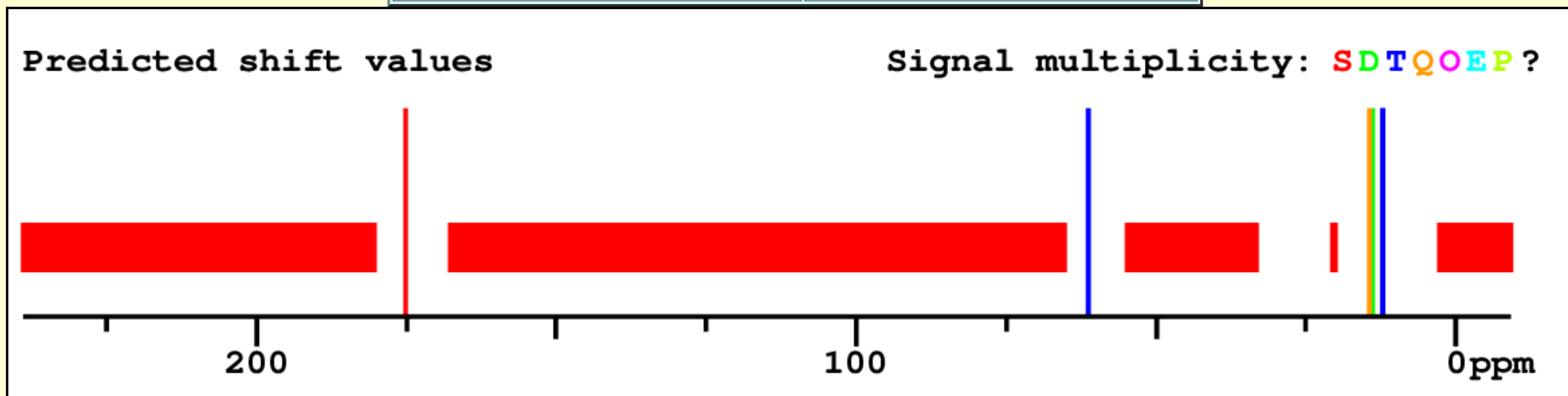
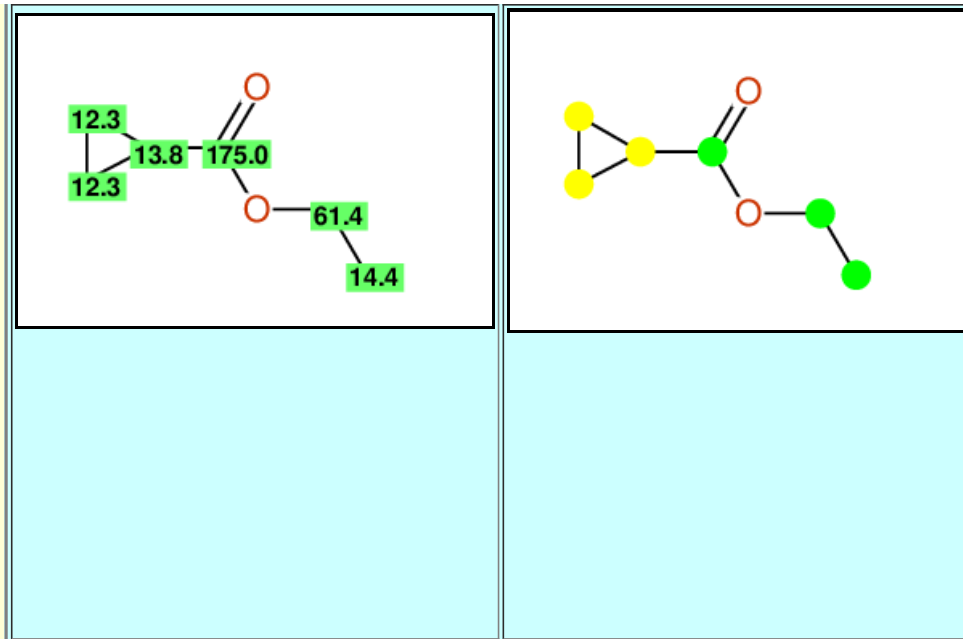


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### Structure Proposal #22

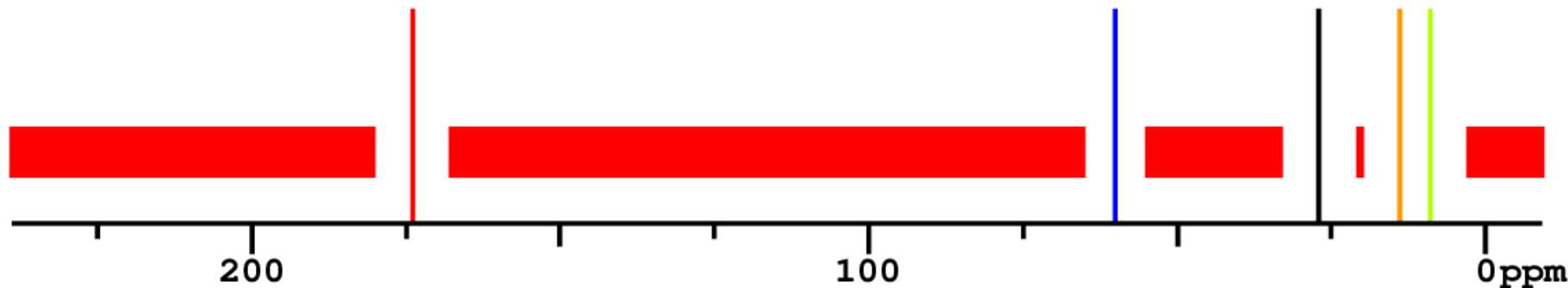
Structure	Similarity Measure
	Deviation = 4.35 ppm Similarity = 75 %  $C_6O_2$  MWT = 104.07  Search Web for this structure:  <a href="#">OARDGAWFHAUQJC</a>
Predicted Chemical Shiftvalues	Matching Map





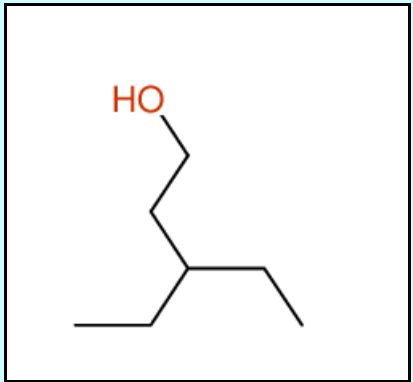
Experimental shift values

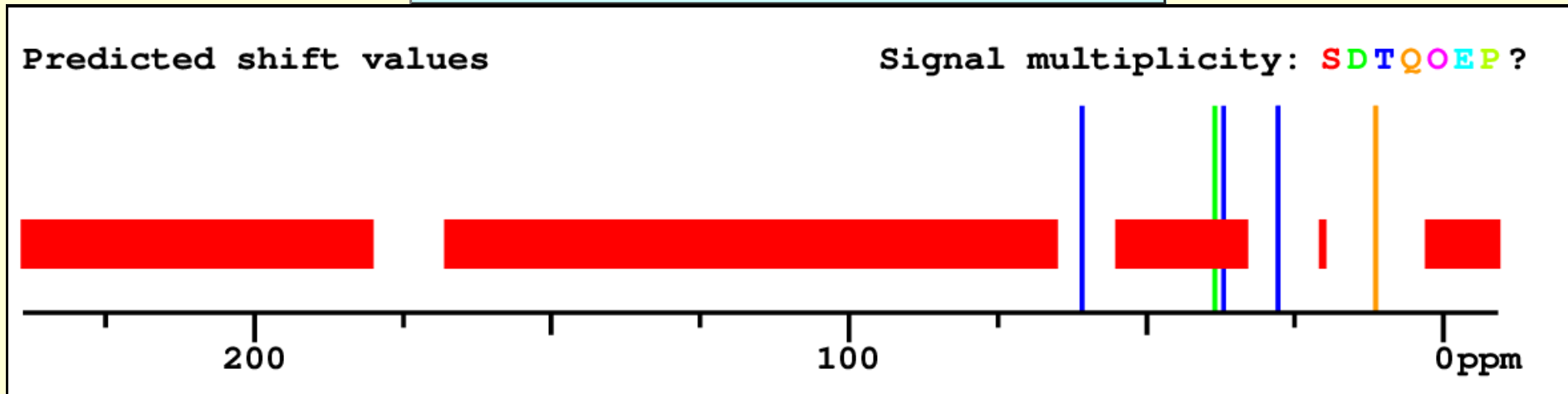
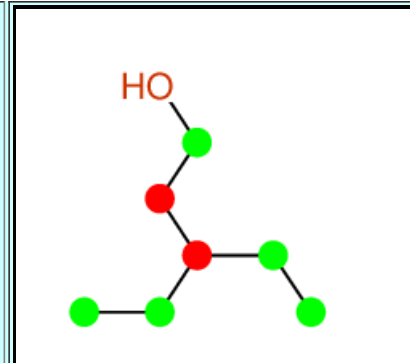
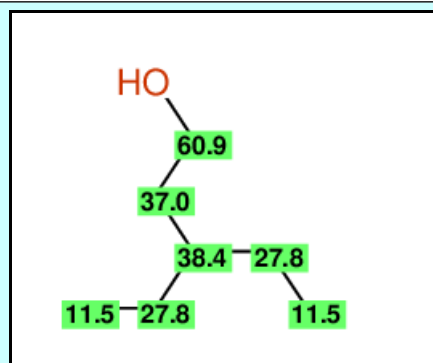
No line in reference: 



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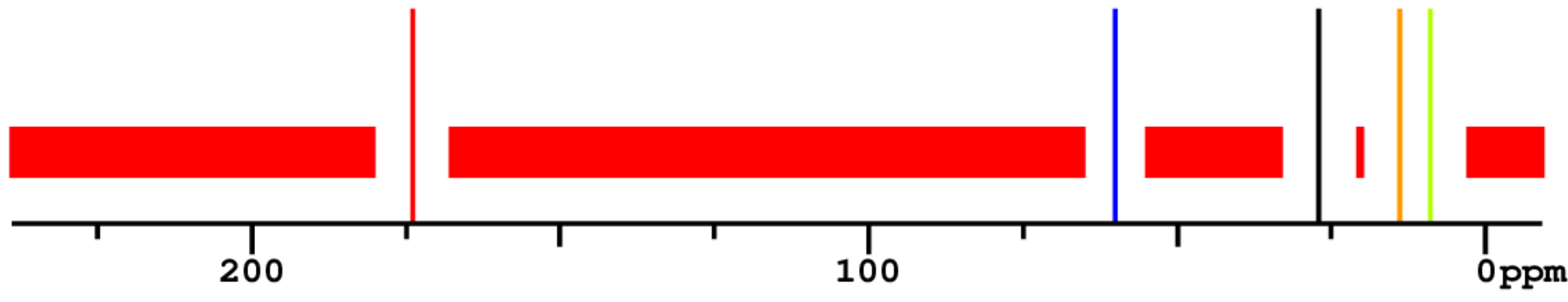
### Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 4.36 ppm Similarity = 71 % (Different pattern)</p> <p>C<sub>7</sub>O</p> <p>MWT = 100.08</p> <p>Search Web for this structure: <a href="#">RLVPCYMDLYVFHH</a></p>
Predicted Chemical Shiftvalues	Matching Map



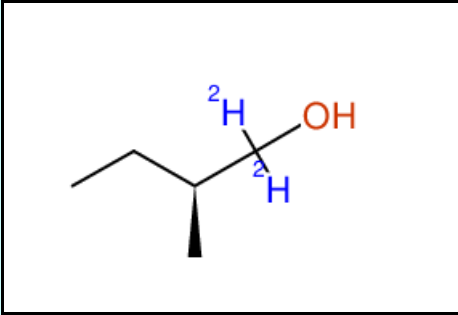
Experimental shift values

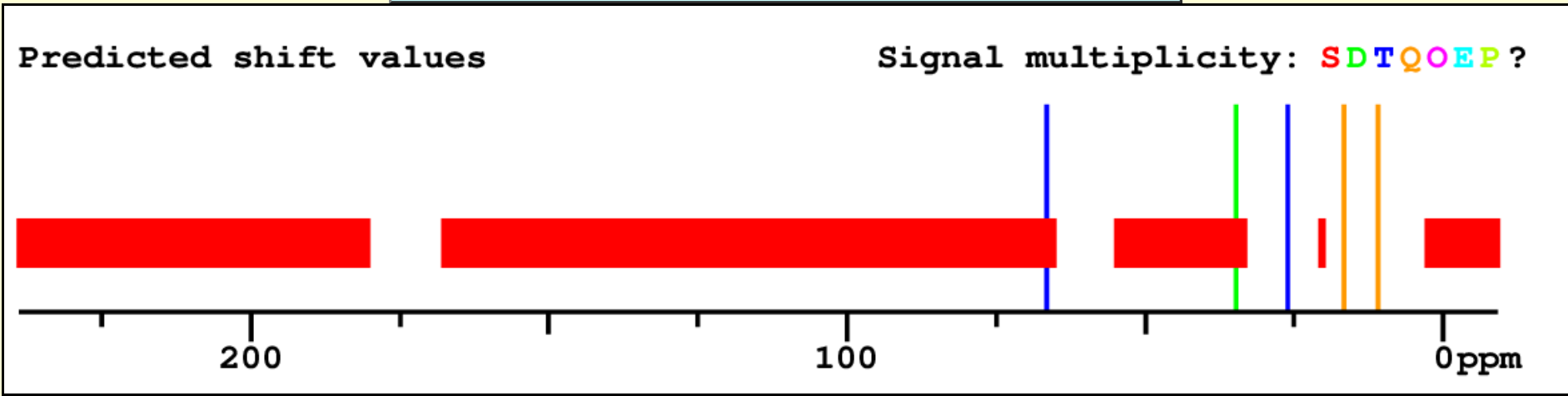
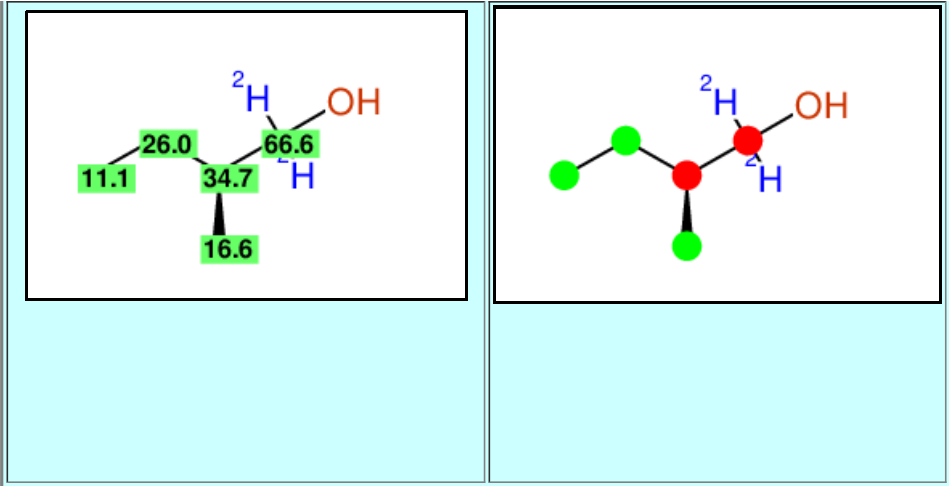
No line in reference: ████████



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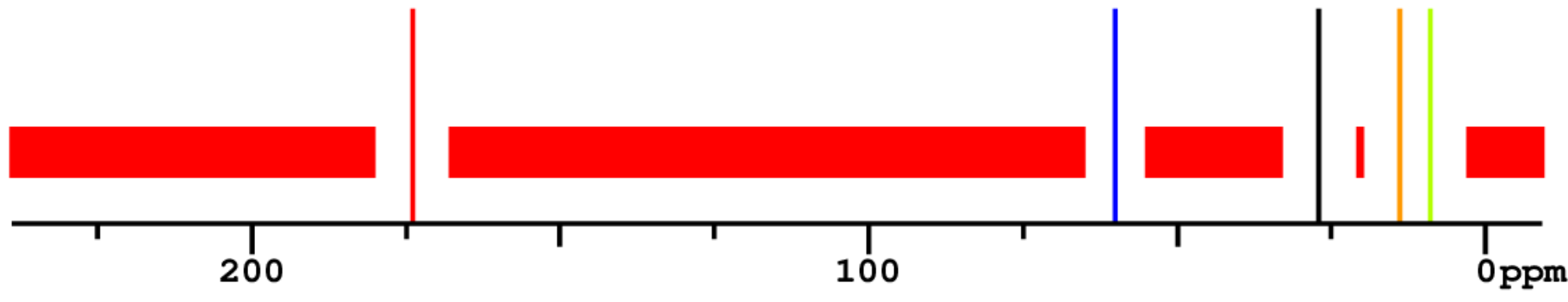
### Structure Proposal #24

Structure	Similarity Measure
	<p>Deviation = 4.42 ppm Similarity = 60 % (Different pattern)</p> <p><math>C_5H_{12}O</math></p> <p>MWT = 90.06</p> <p>Search Web for this structure: <a href="#">QPRQEDXDYOZYLA</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



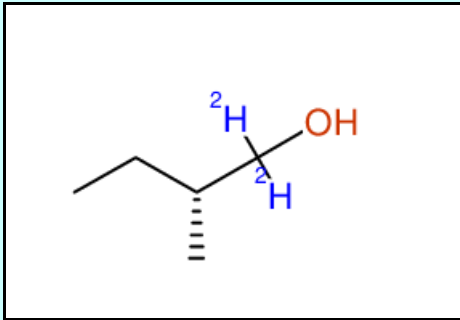
Experimental shift values

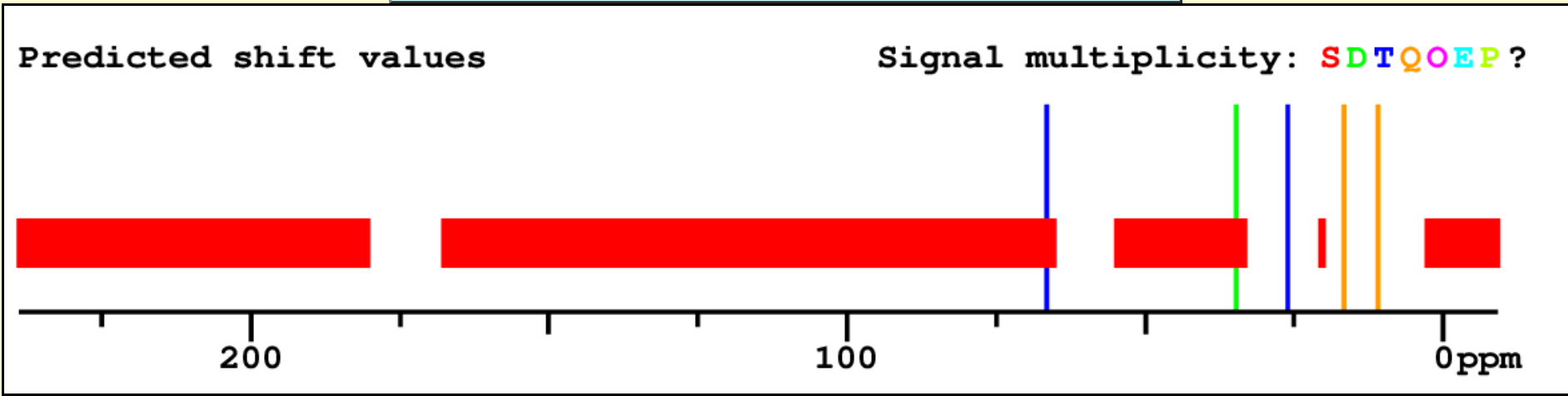
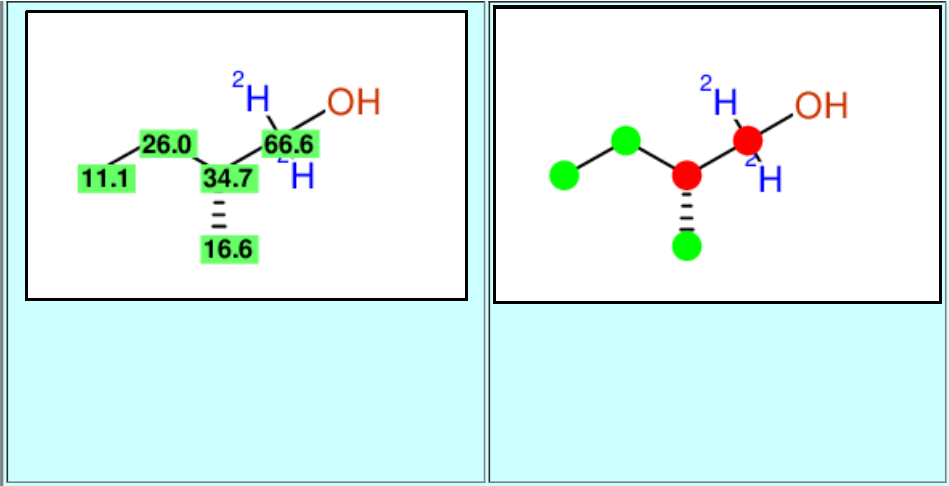
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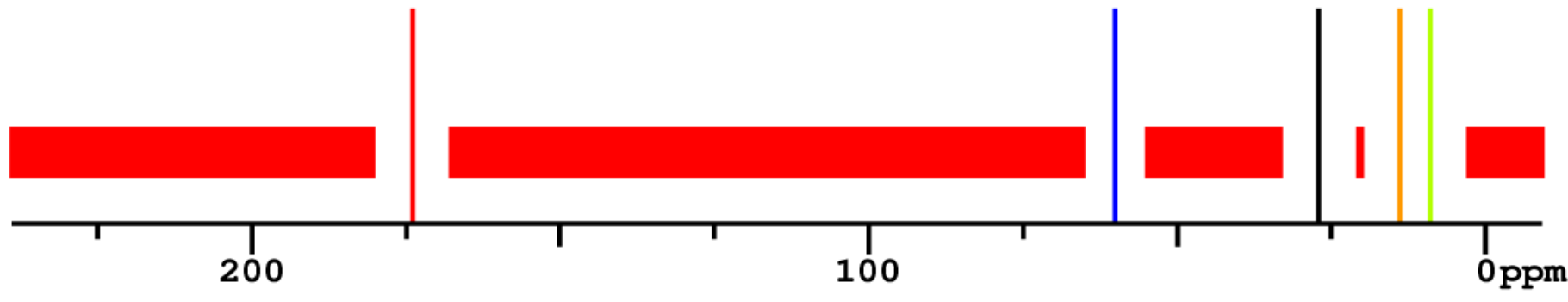
### Structure Proposal #25

Structure	Similarity Measure
	<p>Deviation = 4.42 ppm Similarity = 60 % (Different pattern)</p> <p><math>C_5H_{12}O</math></p> <p>MWT = 90.06</p> <p>Search Web for this structure: <a href="#">QPRQEDXDYOZYLA</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



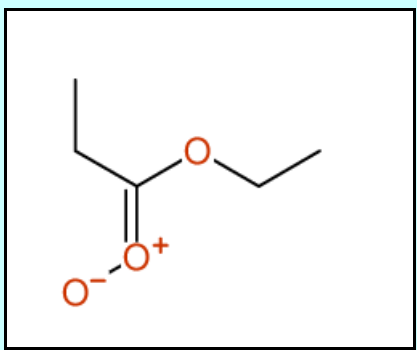
Experimental shift values

No line in reference: ██████████

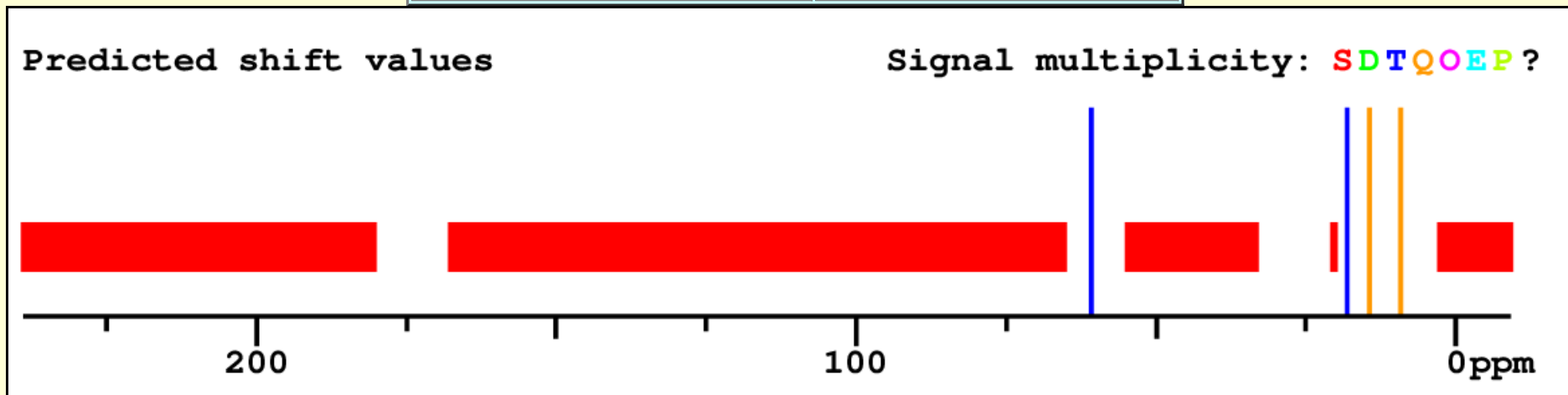
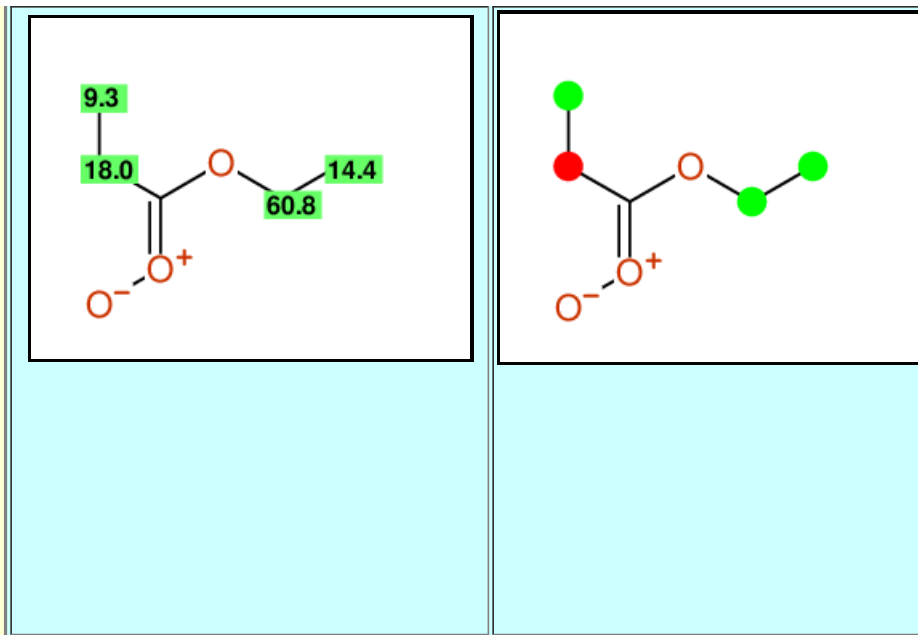


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Structure Proposal #26

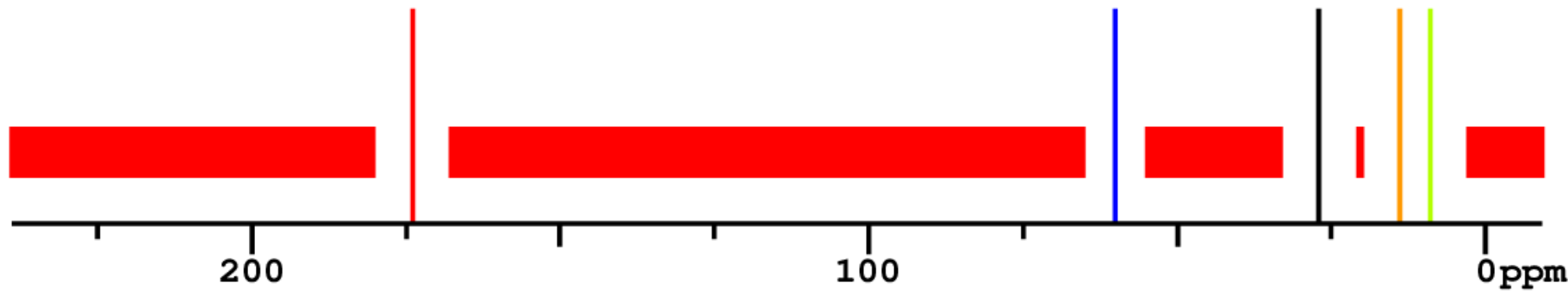
Structure	Similarity Measure
	<p>Deviation = 4.61 ppm Similarity = 75 %</p> <p><math>C_5H_{10}O_3</math></p> <p>MWT = 118.06</p> <p>Search Web for this structure: <a href="#">DIYGJYIIGSAVGQ</a></p>
Predicted Chemical Shiftvalues	Matching Map





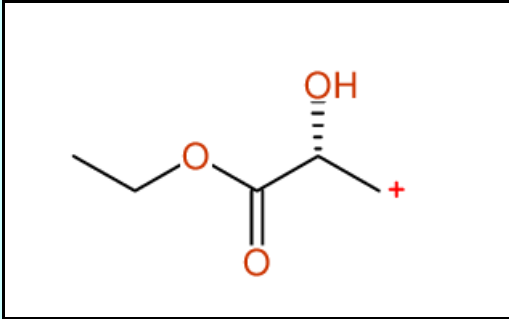
Experimental shift values

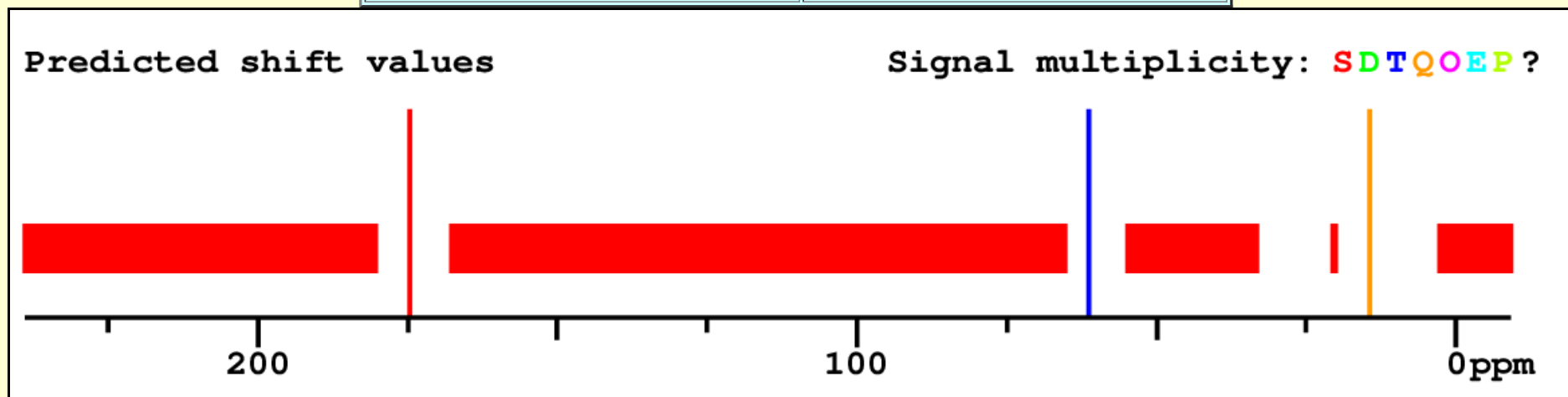
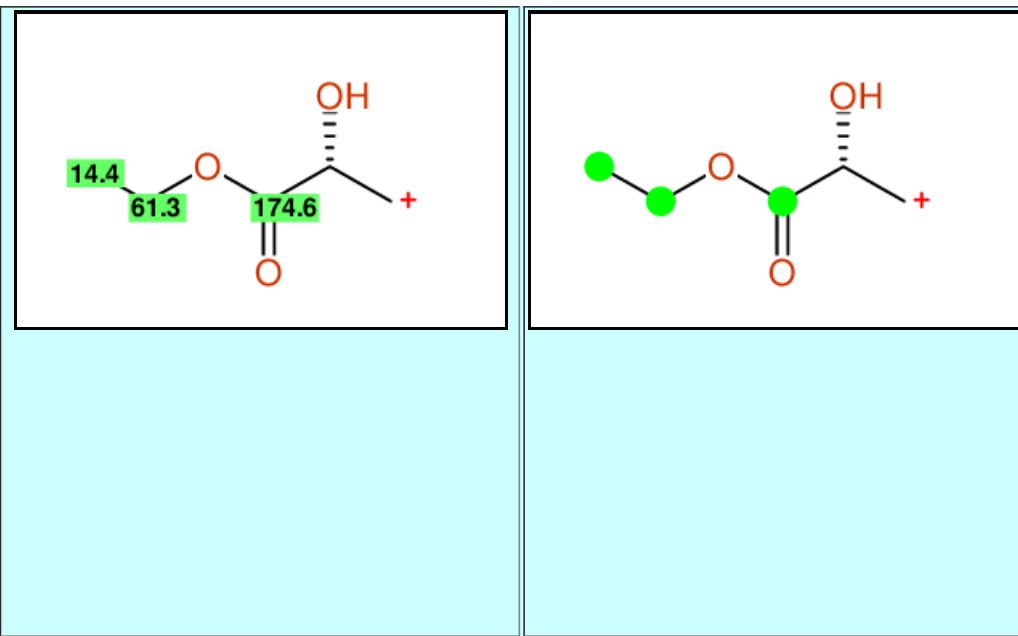
No line in reference: ████████



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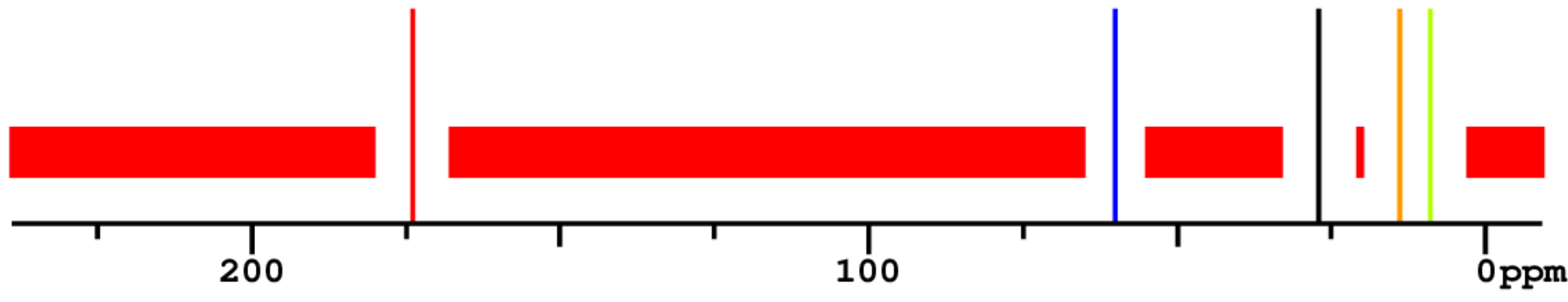
### Structure Proposal #27

Structure	Similarity Measure
 <chem>CCOC(=O)C(O)C</chem>	Deviation = 4.70 ppm Similarity = 100 %  C <sub>5</sub> H <sub>9</sub> O <sub>3</sub>  MWT = 117.06  Search Web for this structure:  <a href="#">SFMRLHJNHWEFDX</a>
Predicted Chemical Shiftvalues	Matching Map



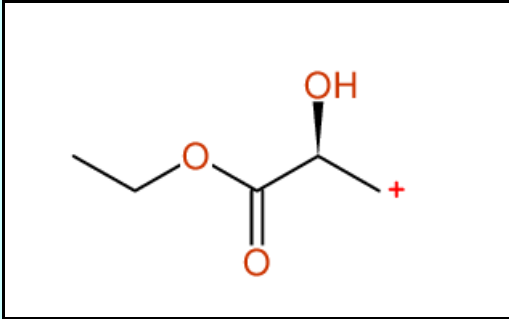
Experimental shift values

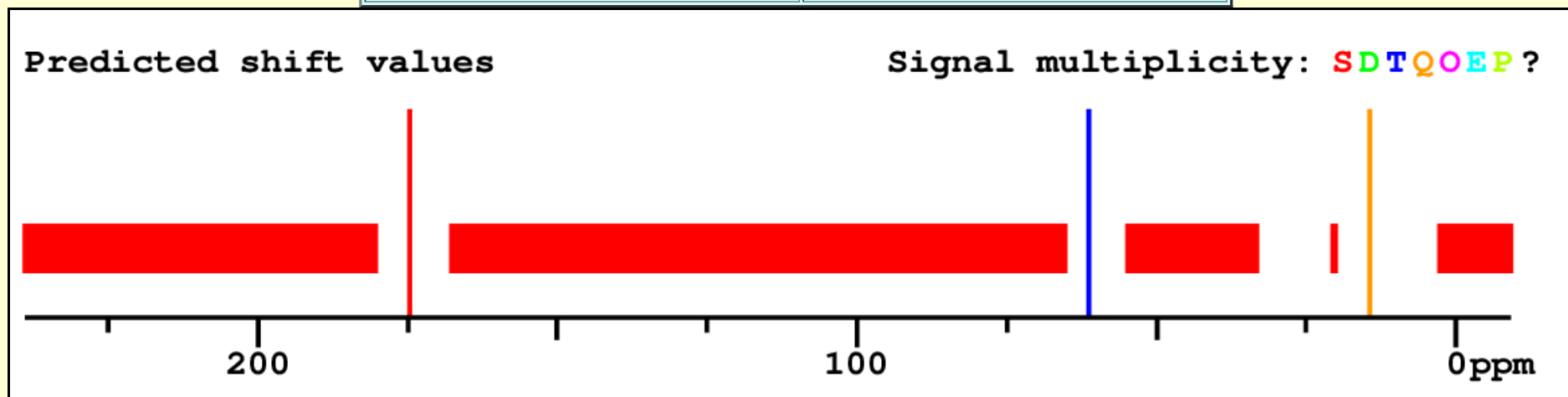
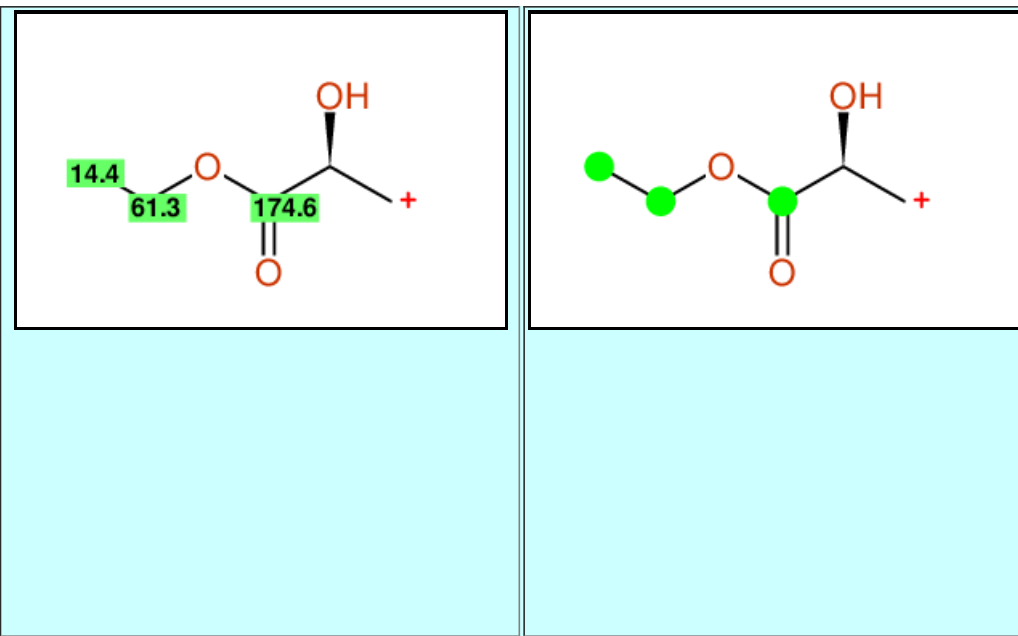
No line in reference: ████████




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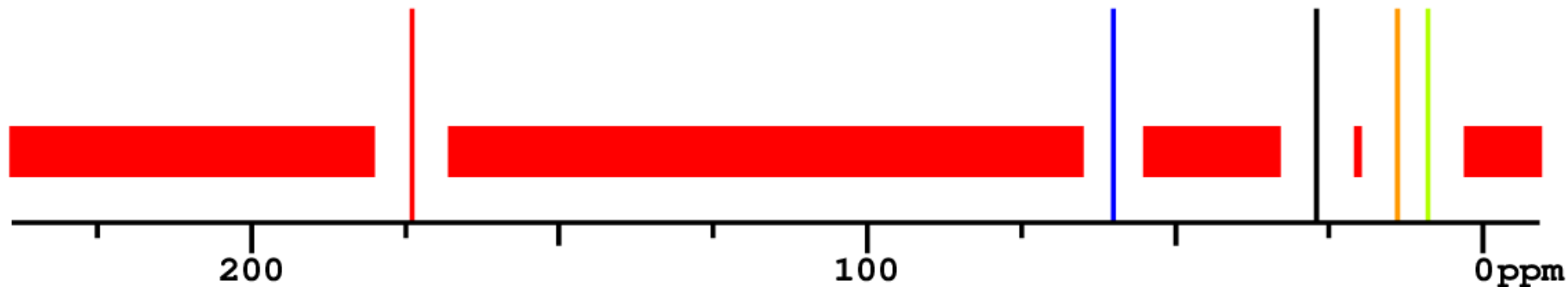
### Structure Proposal #28

Structure	Similarity Measure
 <chem>CCOC(=O)C(O)C</chem>	<p>Deviation = 4.70 ppm Similarity = 100 %</p> <p><math>C_5H_9O_3</math></p> <p>MWT = 117.06</p> <p>Search Web for this structure: <a href="#">SFMRLHJNHWEFDX</a></p>
Predicted Chemical Shiftvalues	Matching Map



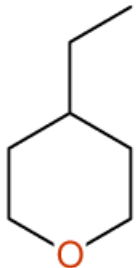
Experimental shift values

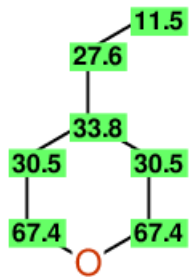
No line in reference: 



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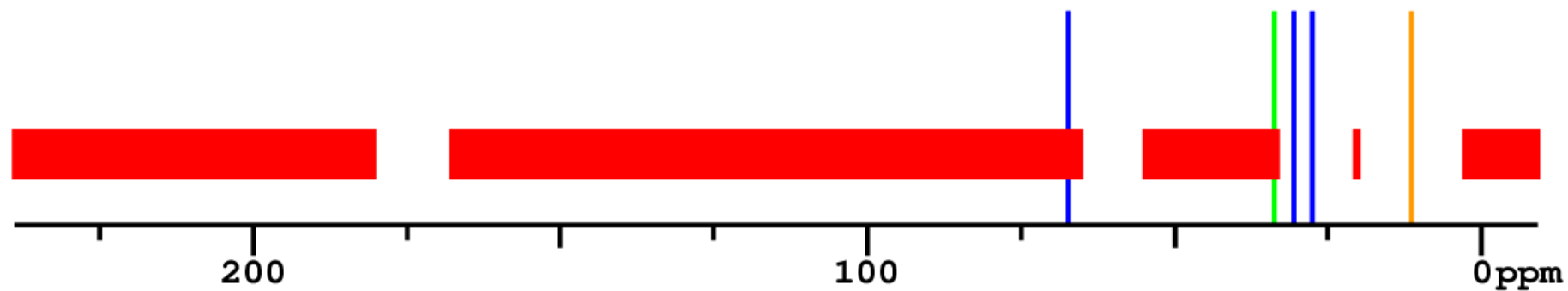
### Structure Proposal #29

Structure	Similarity Measure
	<p>Deviation = 4.72 ppm Similarity = 43 % (Different pattern)</p> <p><math>C_7H_{14}O.H_2</math></p> <p>MWT = 116.08</p> <p>Search Web for this structure: <a href="#">JWWYVYXWJOYSH</a></p>
Predicted Chemical Shiftvalues	Matching Map



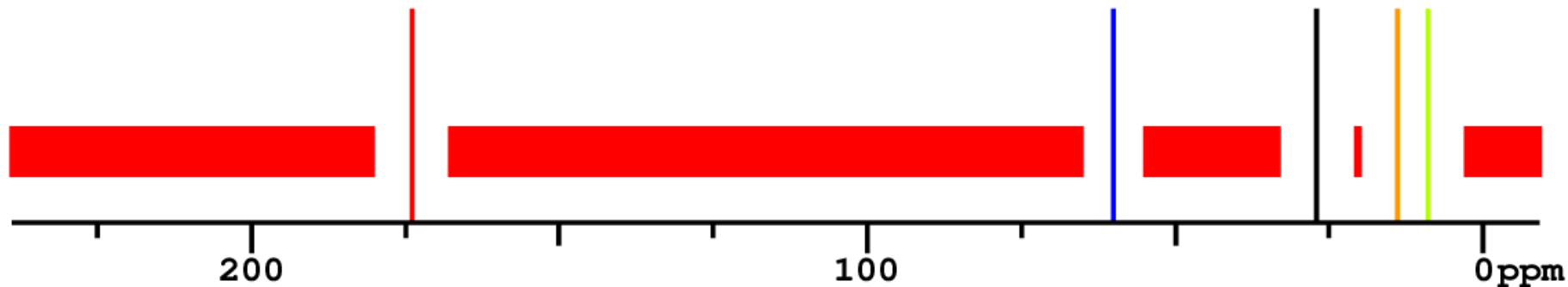
Predicted shift values

Signal multiplicity: S D T Q O E P ?



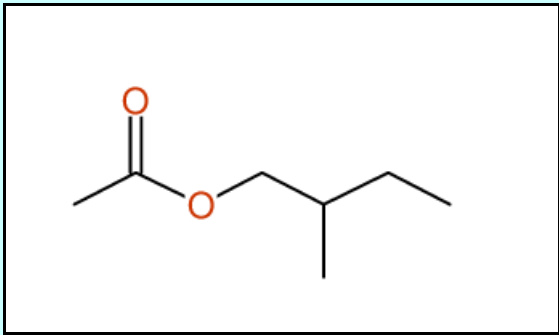
Experimental shift values

No line in reference: 

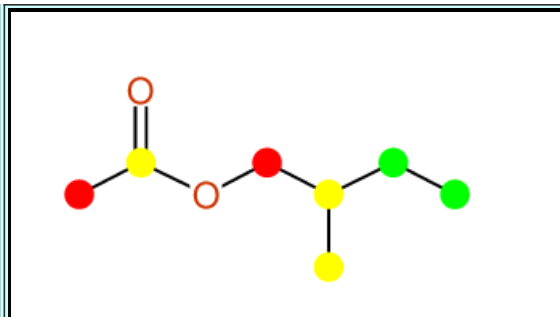
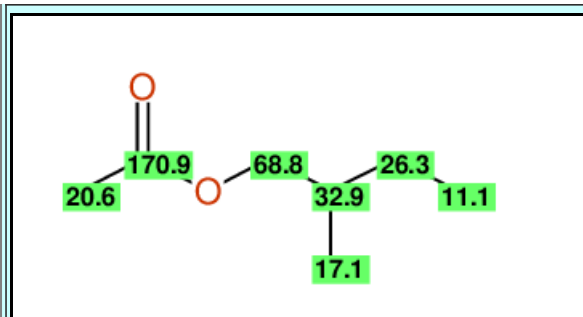


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### Structure Proposal #30

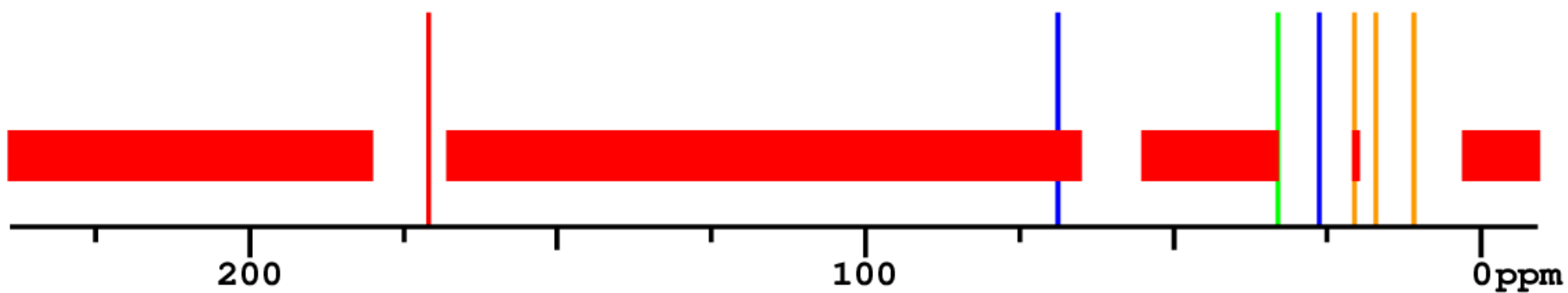
Structure	Similarity Measure
	<p>Deviation = 4.75 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_7O_2</math></p> <p>MWT = 116.08</p> <p>Search Web for this structure: <a href="#">APXBKUAJSWJTRL</a></p>
Predicted Chemical Shiftvalues	Matching Map





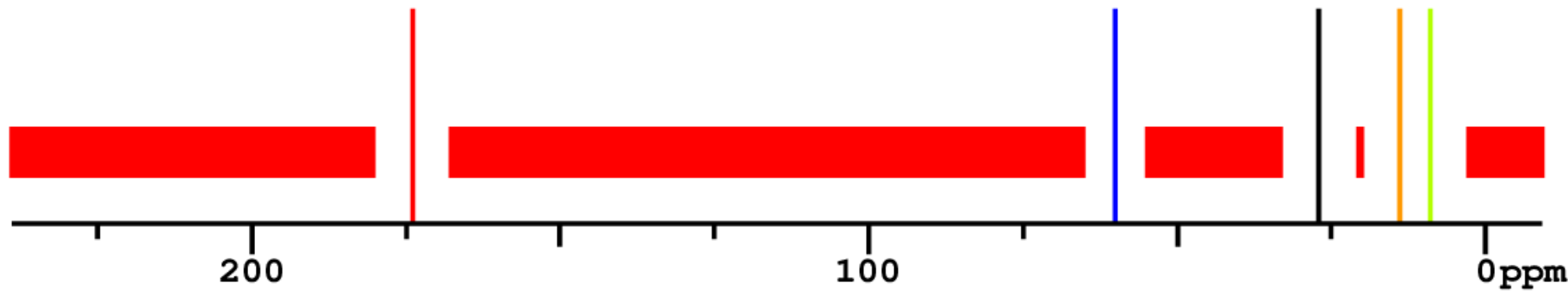
Predicted shift values

Signal multiplicity: S D T Q O E P ?



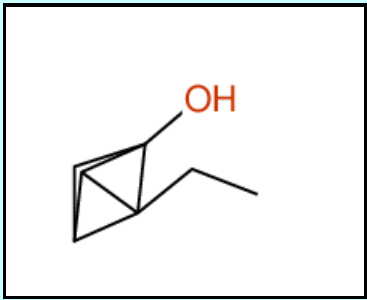
Experimental shift values

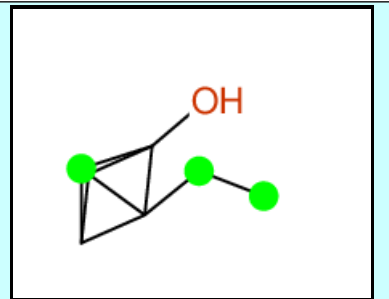
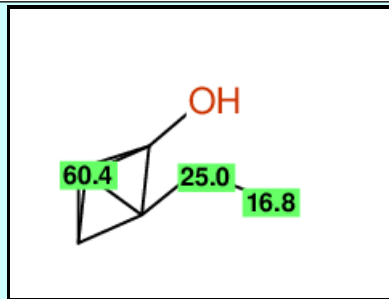
No line in reference: 



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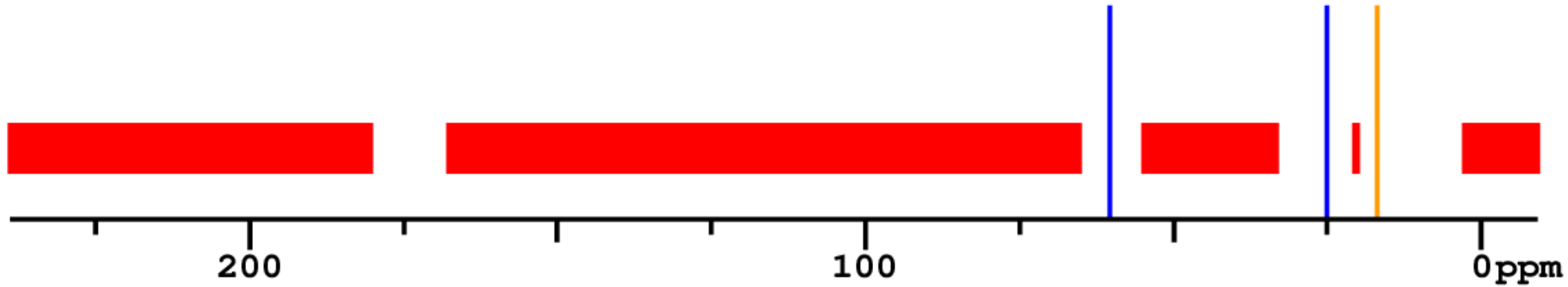
Structure Proposal #31

Structure	Similarity Measure
	<p>Deviation = 4.94 ppm Similarity = 100 %</p> <p><chem>C7H10O</chem></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">JVMWIFFWQQZREC</a></p>
Predicted Chemical Shiftvalues	Matching Map



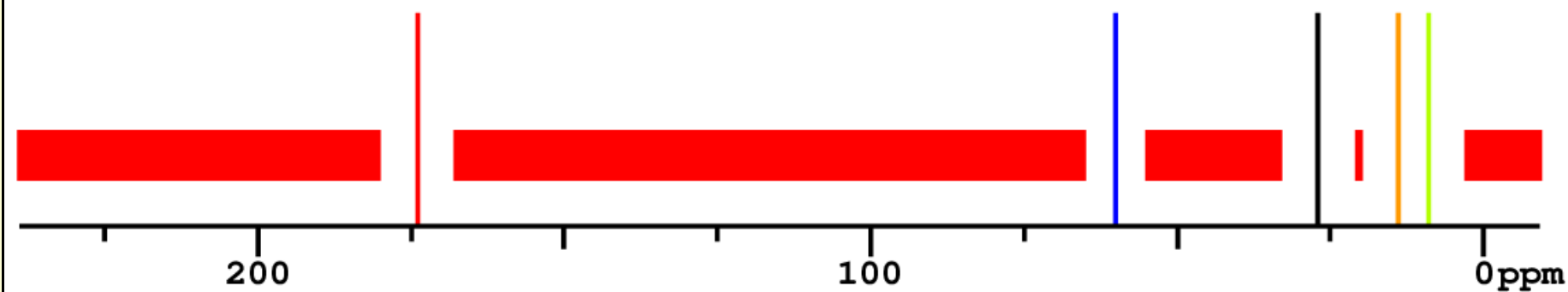
Predicted shift values

Signal multiplicity: S D T Q O E P ?



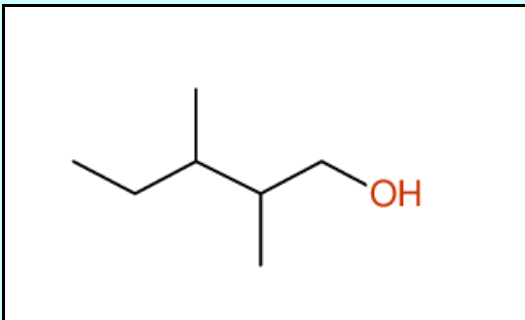
Experimental shift values

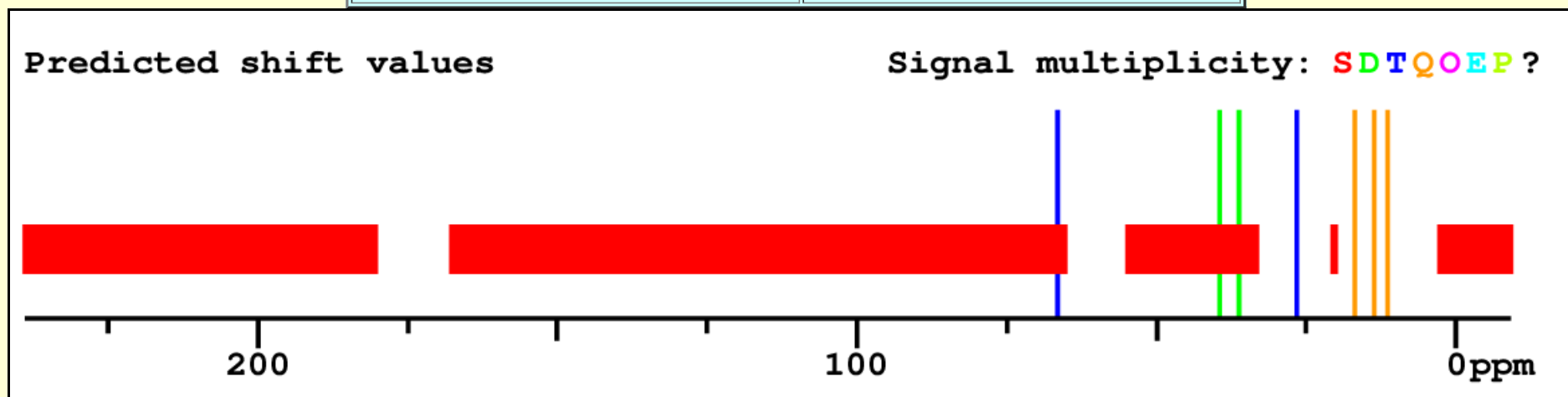
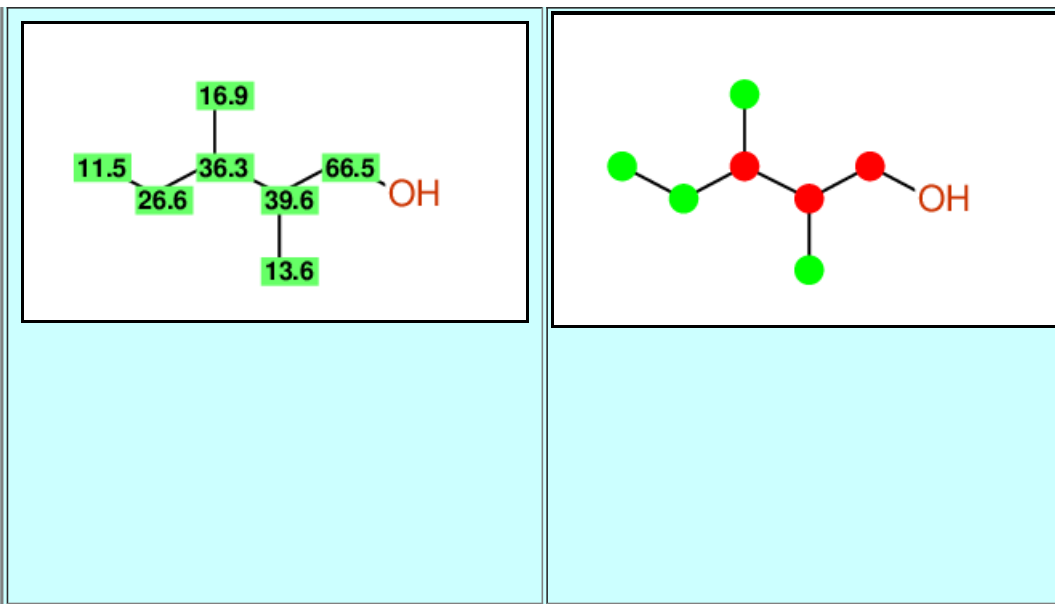
No line in reference: ████████




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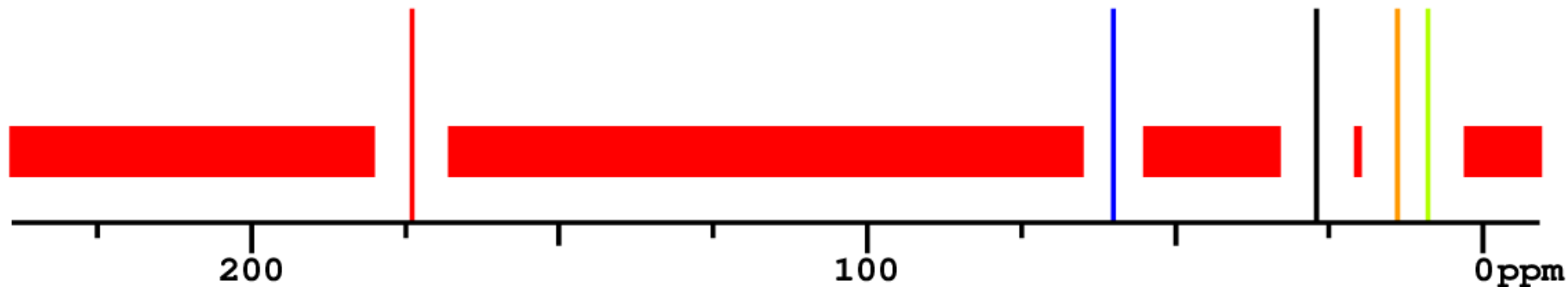
### Structure Proposal #32

Structure	Similarity Measure
 <chem>CC(C)C(O)C(C)CC</chem>	<p>Deviation = 5.20 ppm Similarity = 57 % (Different pattern)</p> <p>C<sub>7</sub>O</p> <p>MWT = 100.08</p> <p>Search Web for this structure: <a href="#">UUESVNYVWMCSAS</a></p>
Predicted Chemical Shiftvalues	Matching Map



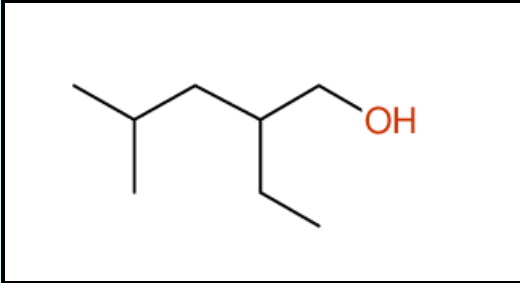
Experimental shift values

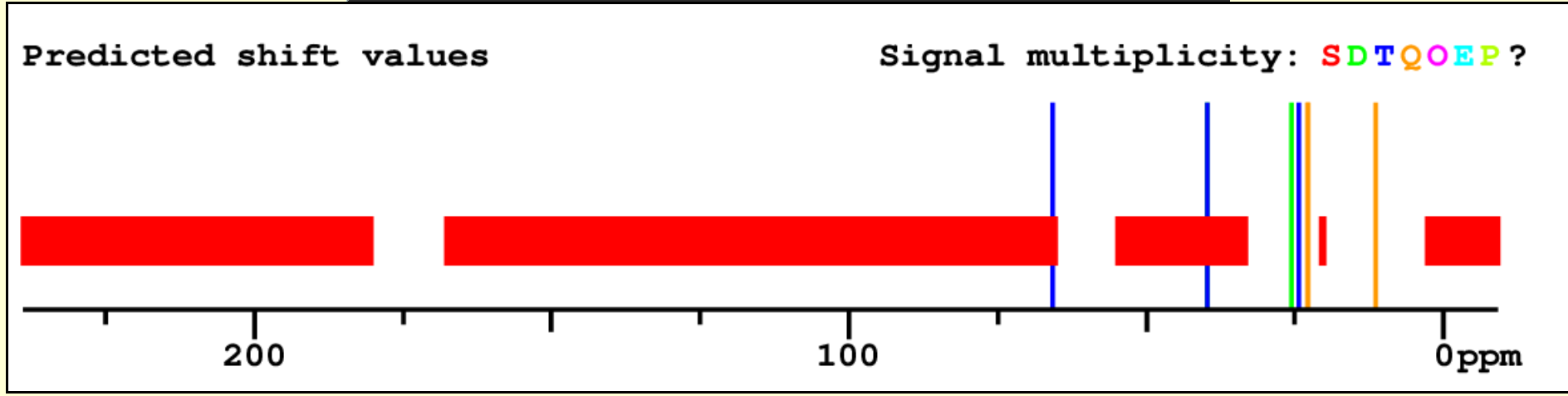
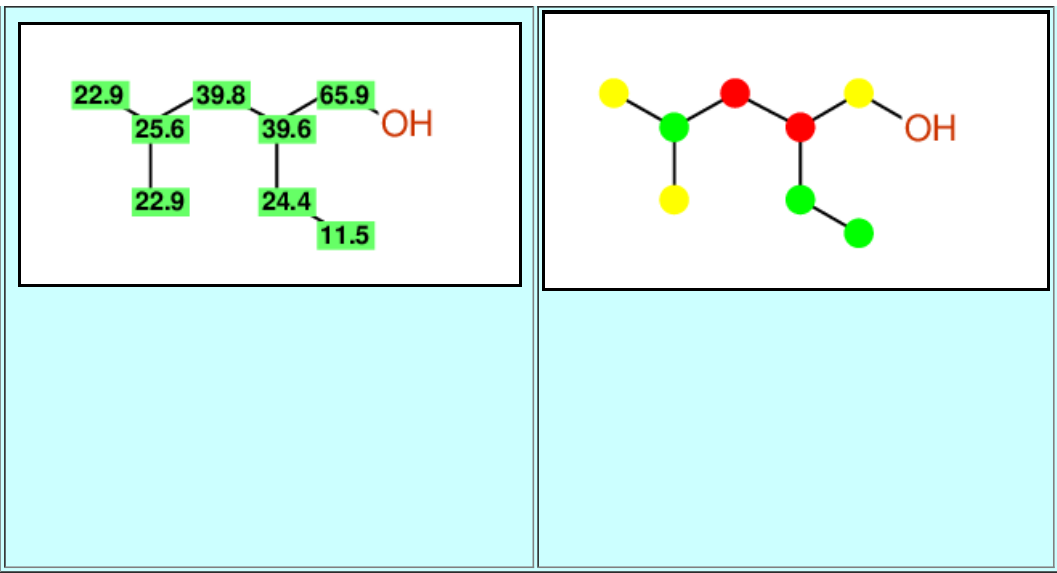
No line in reference: 



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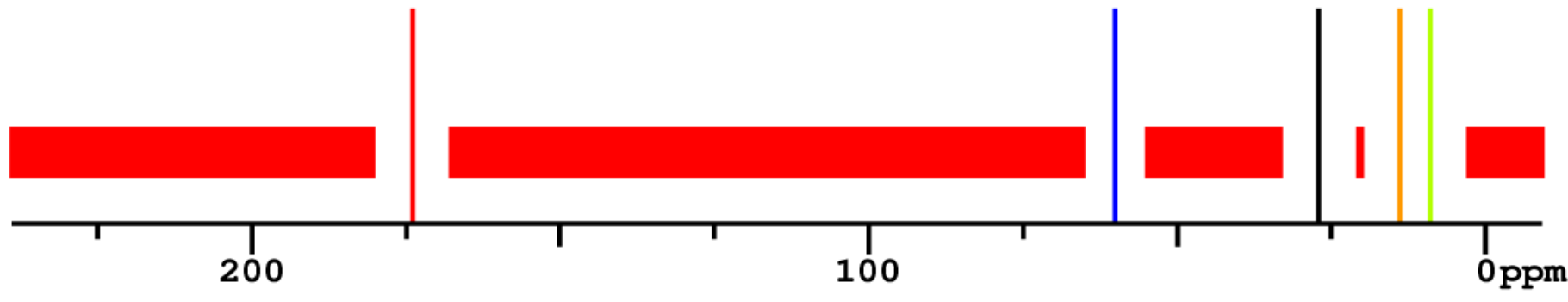
### Structure Proposal #33

Structure	Similarity Measure
	<p>Deviation = 5.49 ppm Similarity = 56 % (Different pattern)</p> <p>C<sub>8</sub>O</p> <p>MWT = 112.09</p> <p>Search Web for this structure: <a href="#">IDWODMMAHQBYRU</a></p>
Predicted Chemical Shiftvalues	Matching Map



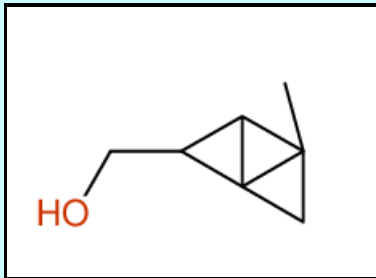
Experimental shift values

No line in reference: 

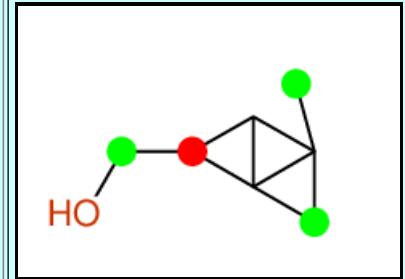
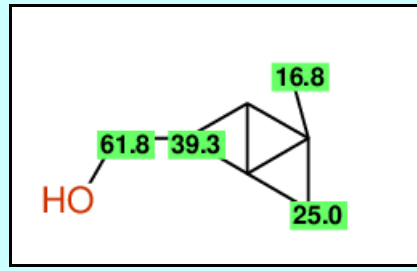


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### Structure Proposal #34

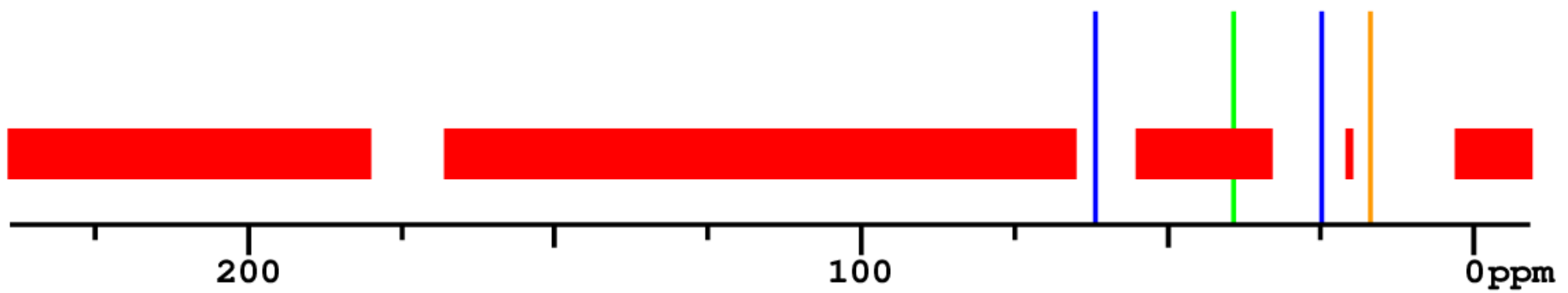
Structure	Similarity Measure
	<p>Deviation = 5.60 ppm Similarity = 75 % (Different pattern)</p> <p><math>C_7H_{10}O</math></p> <p>MWT = 110.08</p> <p>Search Web for this structure: <a href="#">JYMZYTRPGHEQSC</a></p>
Predicted Chemical Shiftvalues	Matching Map





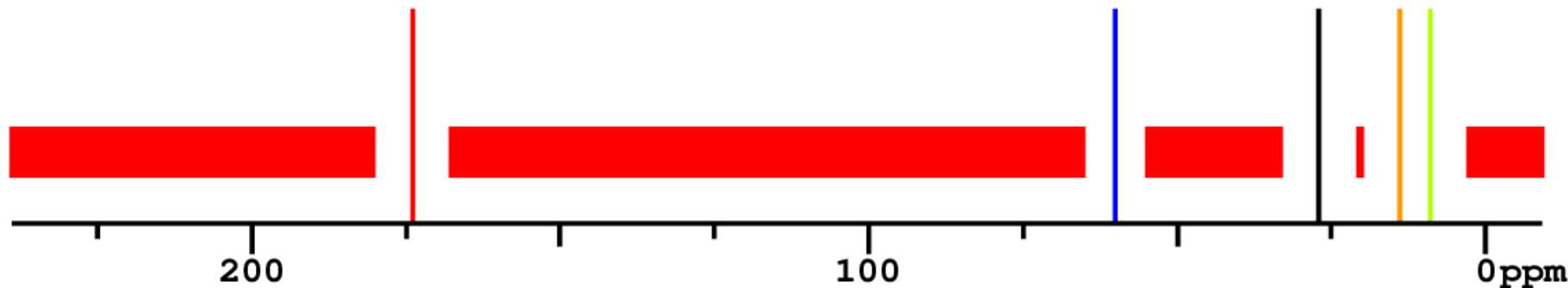
Predicted shift values

Signal multiplicity: S D T Q O E P ?



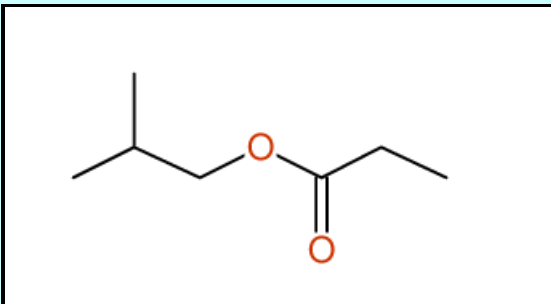
Experimental shift values

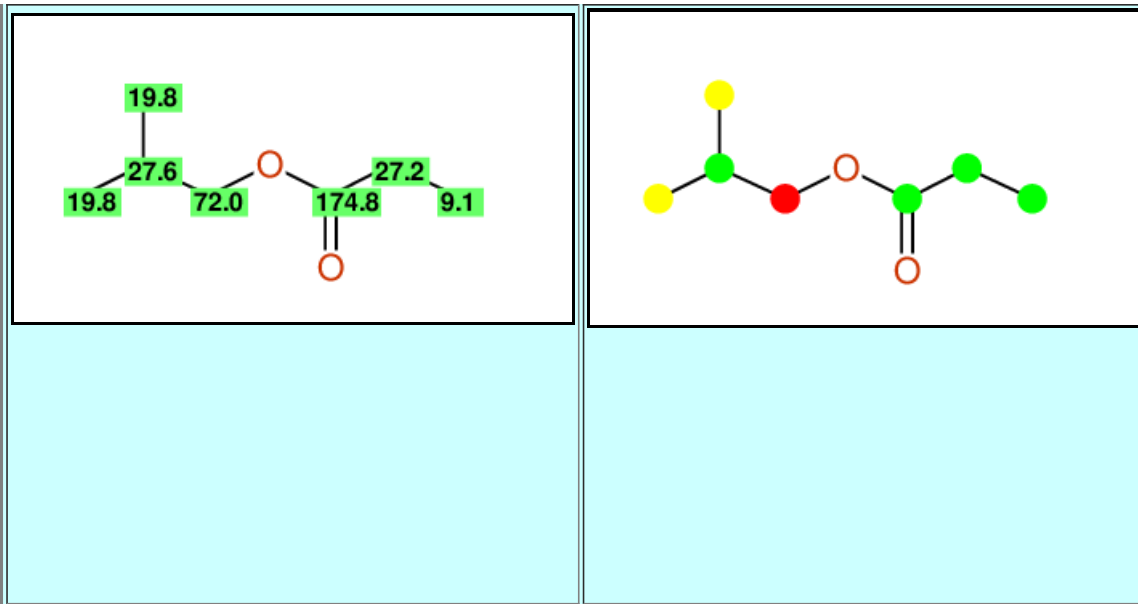
No line in reference: 



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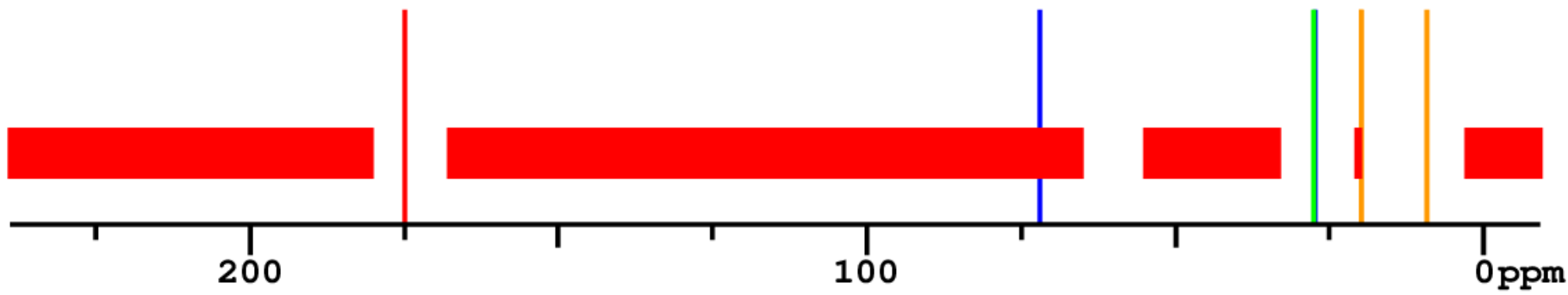
### Structure Proposal #35

Structure	Similarity Measure
	<p>Deviation = 5.66 ppm Similarity = 71 % (Different pattern)</p> <p><math>C_7O_2</math></p> <p>MWT = 116.08</p> <p>Search Web for this structure: <a href="#">CPOGEOGDMOTURU</a></p>
Predicted Chemical Shiftvalues	Matching Map



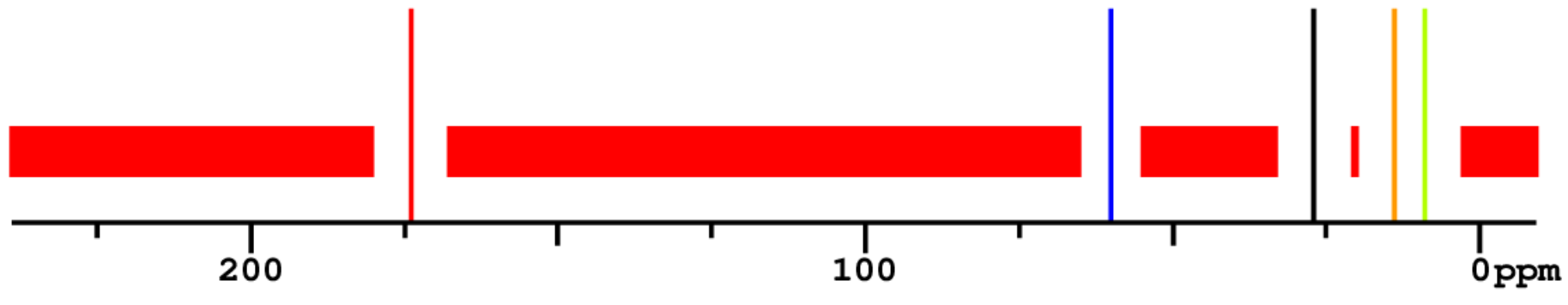
Predicted shift values

Signal multiplicity: S D T Q O E P ?



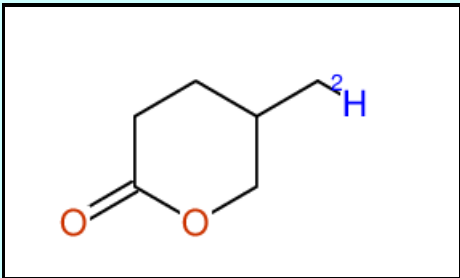
Experimental shift values

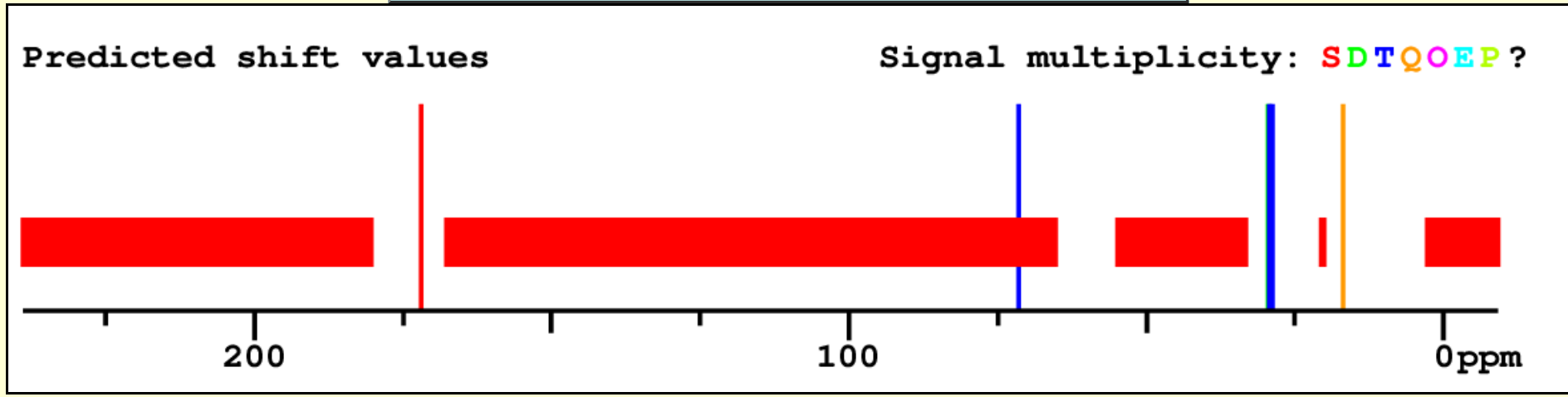
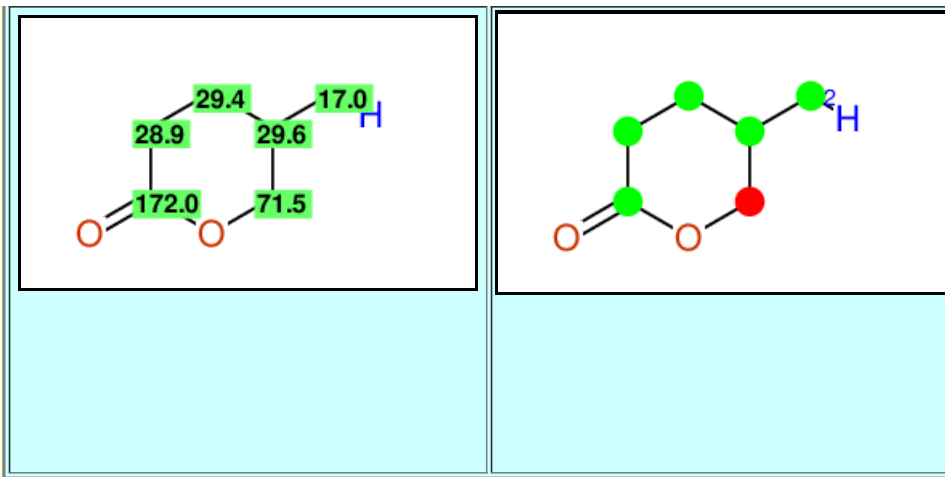
No line in reference: 



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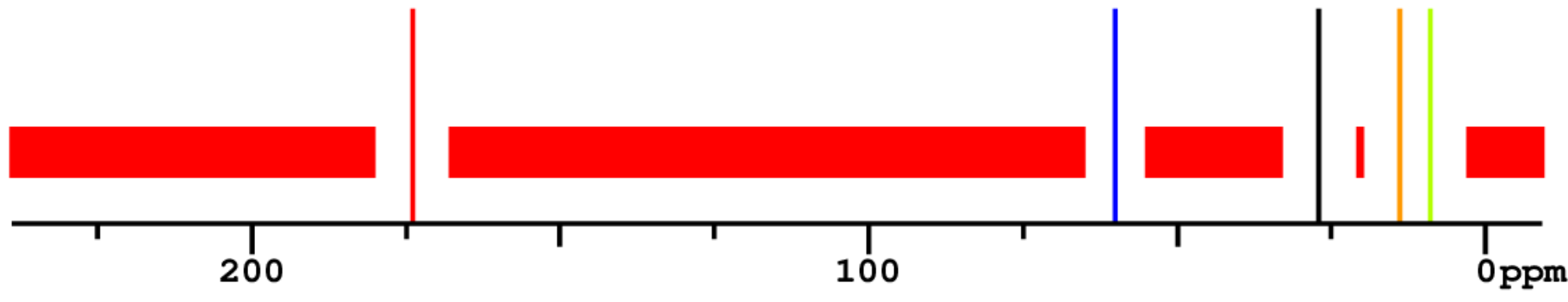
### Structure Proposal #36

Structure	Similarity Measure
	<p>Deviation = 5.85 ppm Similarity = 83 % (Different pattern)</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 115.07</p> <p>Search Web for this structure: <a href="#">GQUBDAOKWZLWDI</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



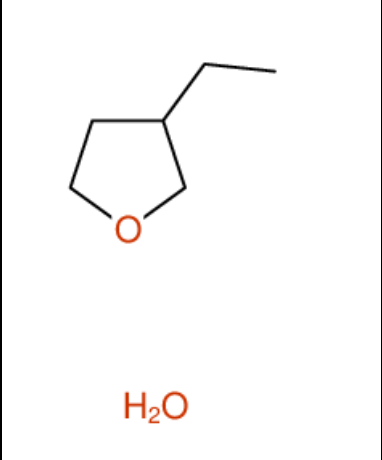
Experimental shift values

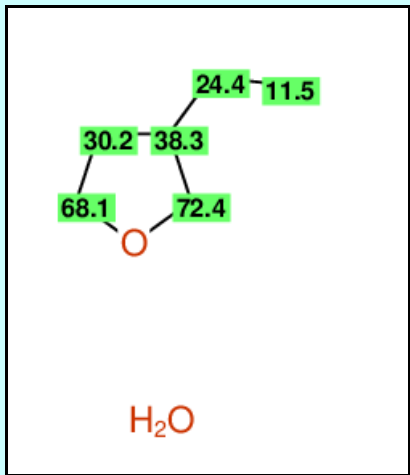
No line in reference: 



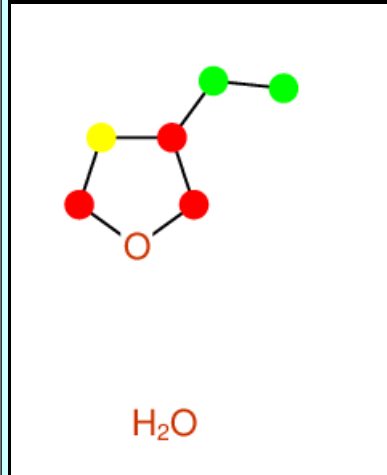
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Structure Proposal #37

Structure	Similarity Measure
 <p><chem>CCOC1CCOC1</chem></p> <p>H<sub>2</sub>O</p>	<p>Deviation = 6.27 ppm Similarity = 42 % (Different pattern)</p> <p>C<sub>6</sub>H<sub>12</sub>O.H<sub>2</sub>O</p> <p>MWT = 118.07</p> <p>Search Web for this structure: <a href="#">RSKEUFGEOZQDHE</a></p>
Predicted Chemical Shiftvalues	Matching Map



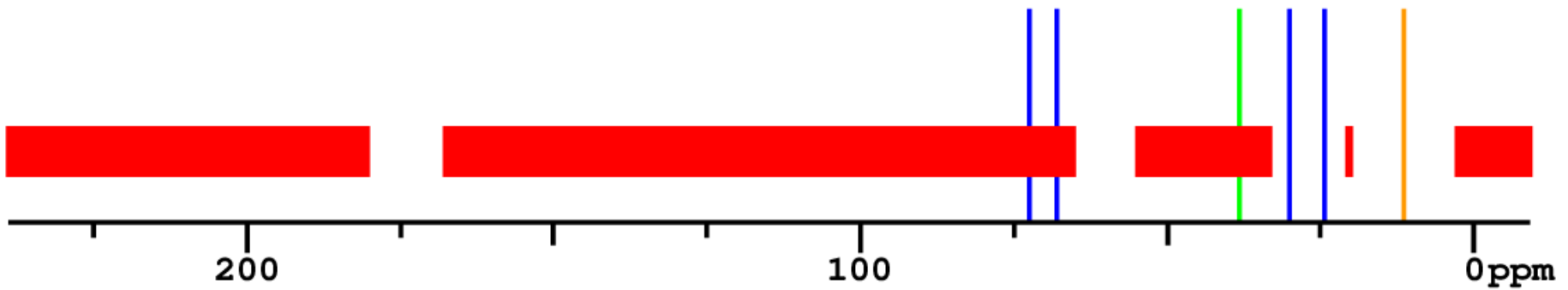
$H_2O$



$H_2O$

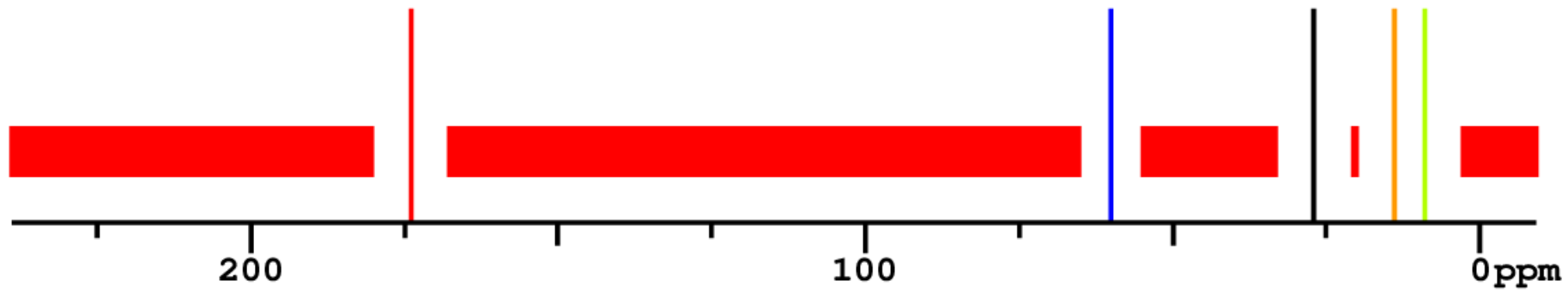
Predicted shift values

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



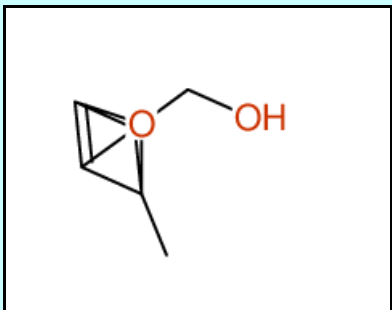
Experimental shift values

No line in reference: 

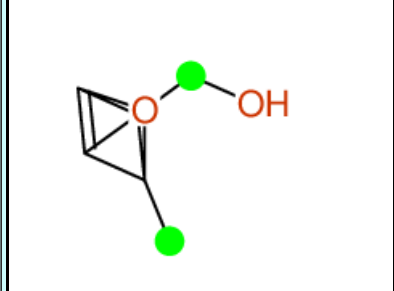
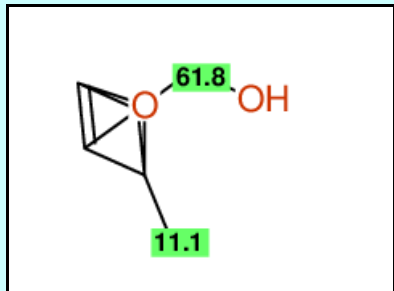


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### Structure Proposal #38

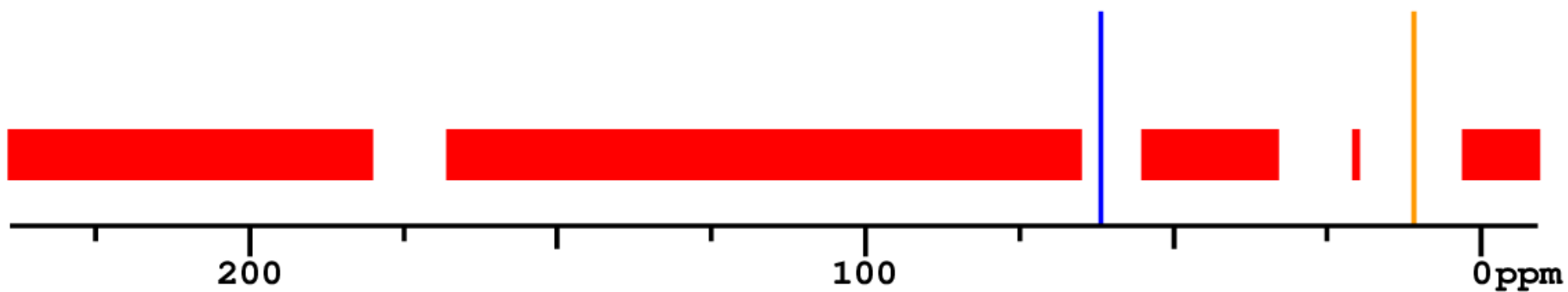
Structure	Similarity Measure
	Deviation = 6.35 ppm Similarity = 100 %  $C_6H_6O_2$  MWT = 110.07  Search Web for this structure: <a href="#">ISLZYQGILDDIOB</a>
Predicted Chemical Shiftvalues	Matching Map





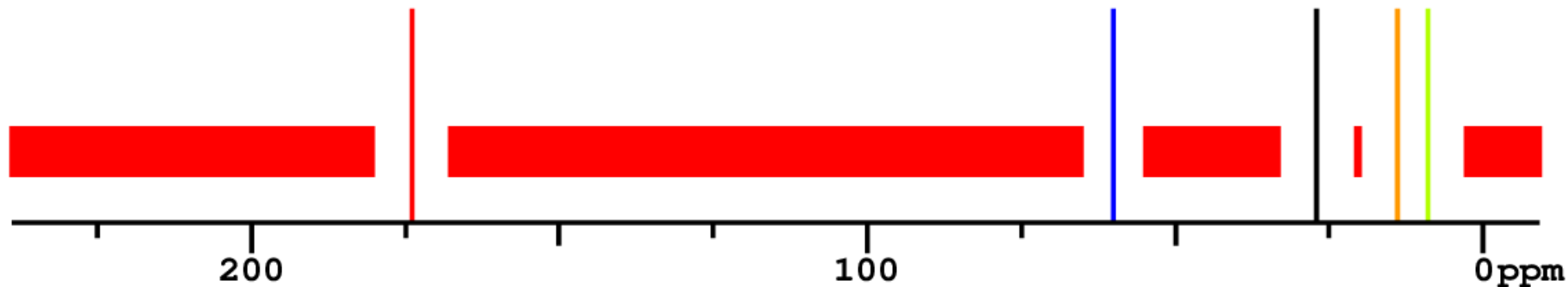
Predicted shift values

Signal multiplicity: S D T Q O E P ?



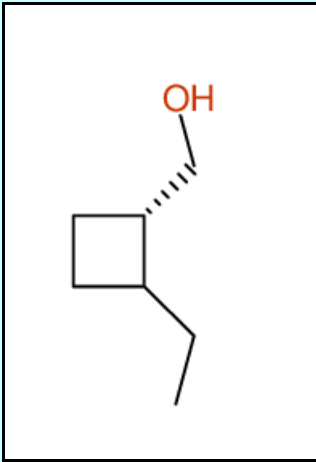
Experimental shift values

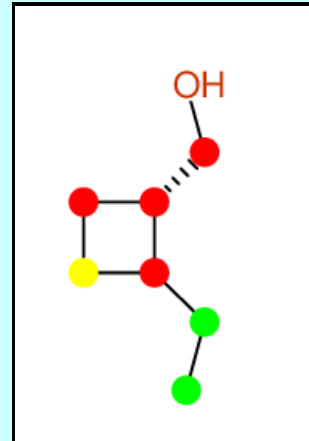
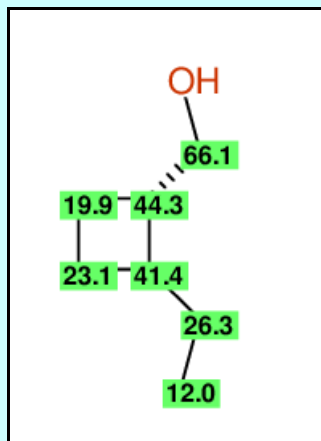
No line in reference: ████████



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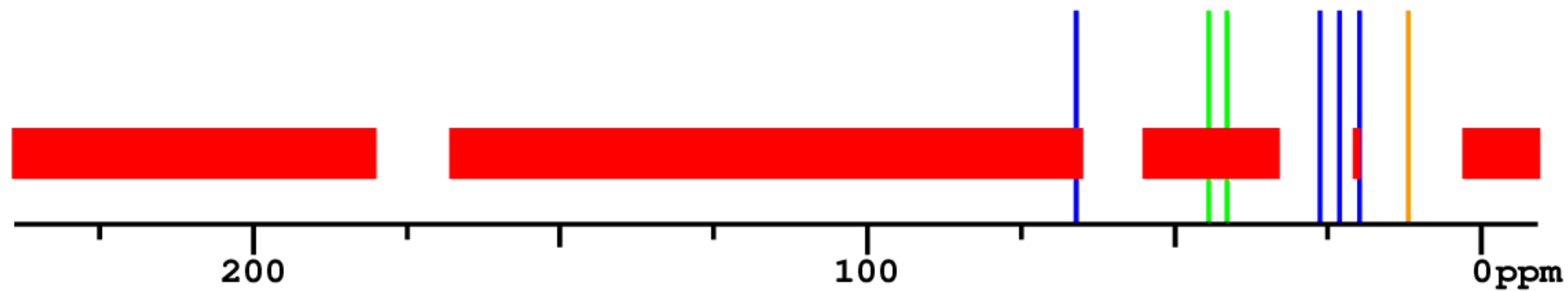
### Structure Proposal #39

Structure	Similarity Measure
	<p>Deviation = 6.64 ppm Similarity = 36 % (Different pattern)</p> <p><math>C_7H_{14}O</math></p> <p>MWT = 114.08</p> <p>Search Web for this structure: <a href="#">HWPQBLRHKPOPJG</a></p>
Predicted Chemical Shiftvalues	Matching Map



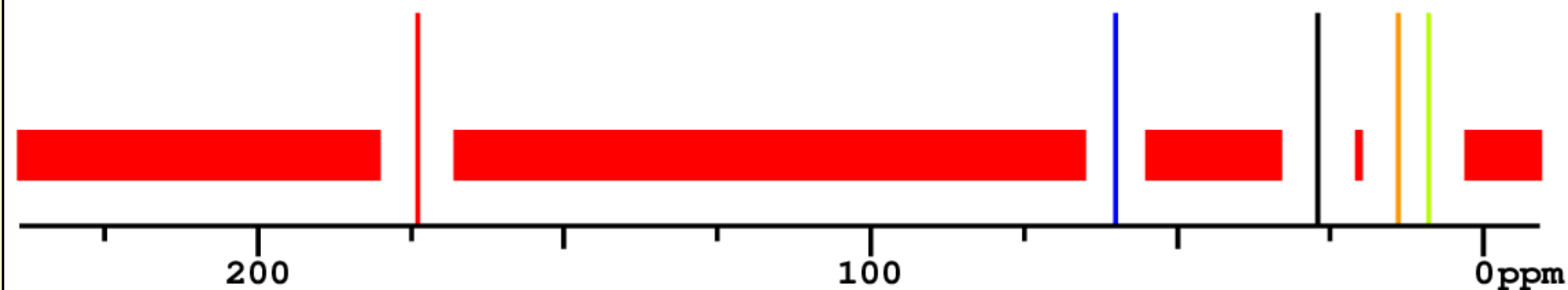
Predicted shift values

Signal multiplicity: S D T Q O E P ?



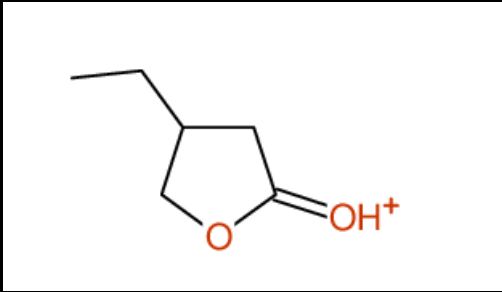
Experimental shift values

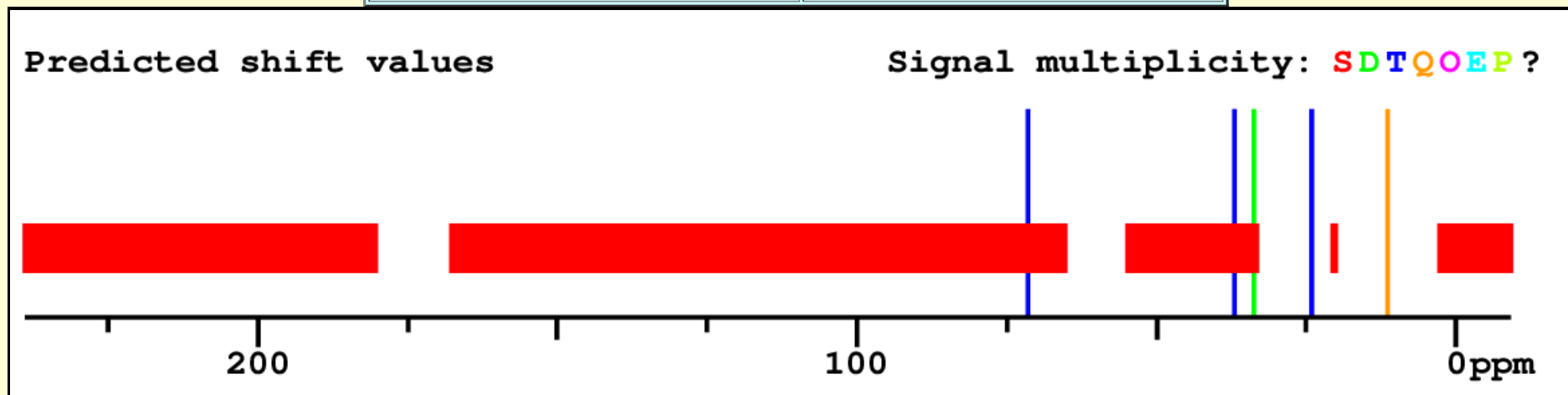
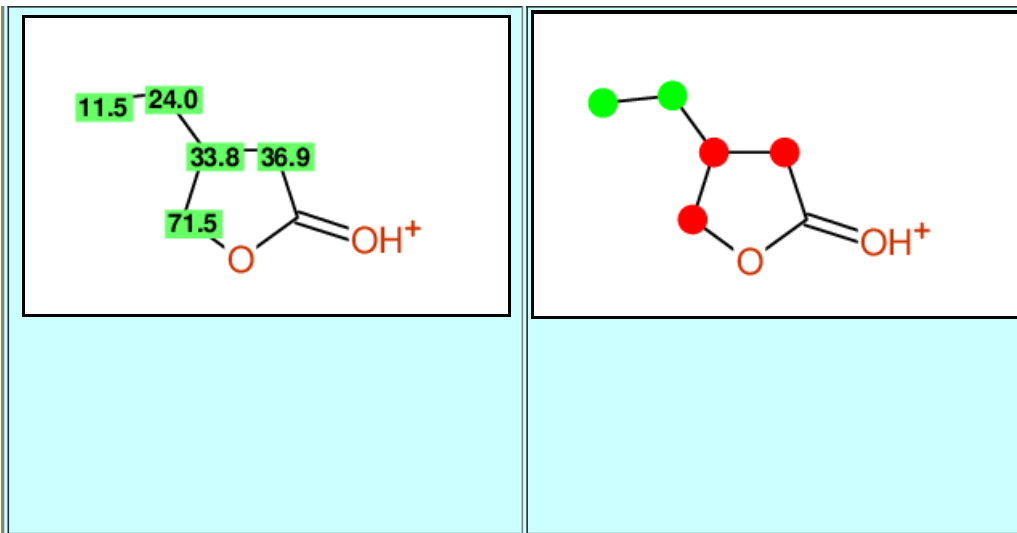
No line in reference: 



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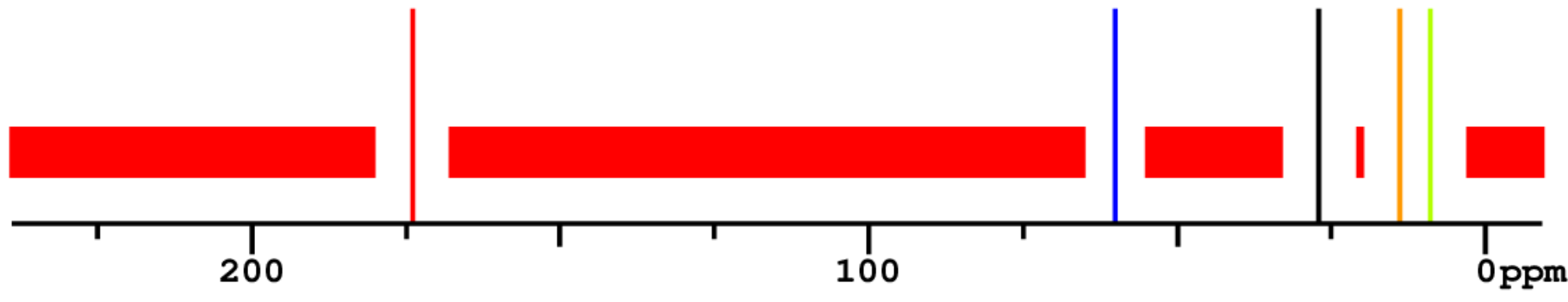
### Structure Proposal #40

Structure	Similarity Measure
	<p>Deviation = 6.69 ppm Similarity = 40 % (Different pattern)</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.07</p> <p>Search Web for this structure: <a href="#">MDQZVJSUBKPTHG</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



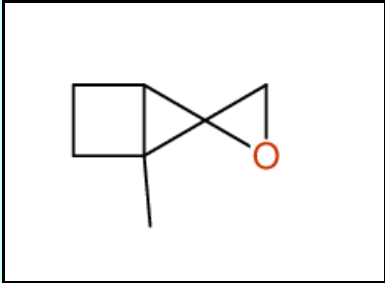
Experimental shift values

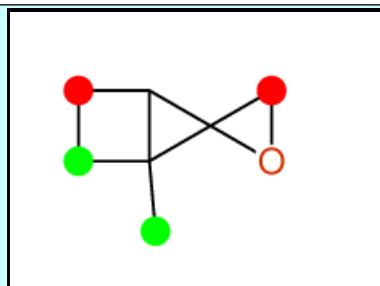
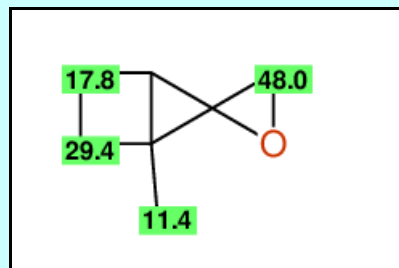
No line in reference: 



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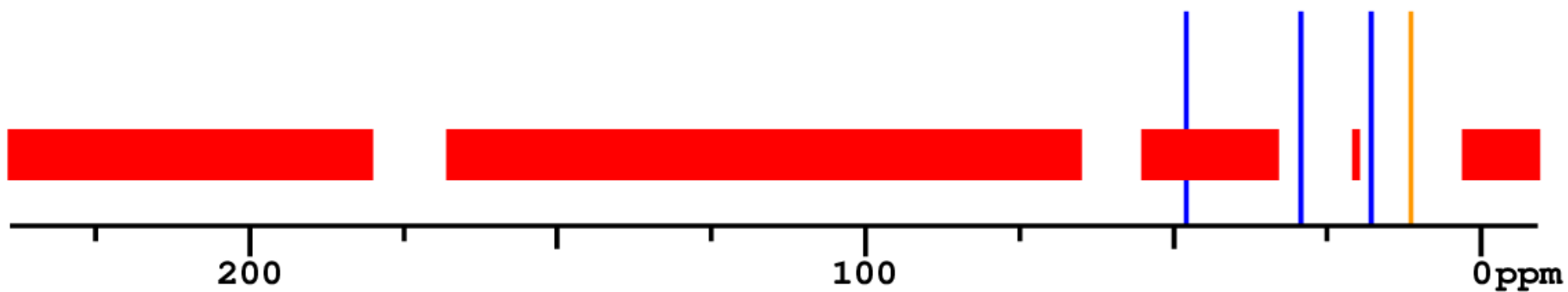
### Structure Proposal #41

Structure	Similarity Measure
	<p>Deviation = 6.75 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="#">LIKWSDHCOZEJBT</a></p>
Predicted Chemical Shiftvalues	Matching Map



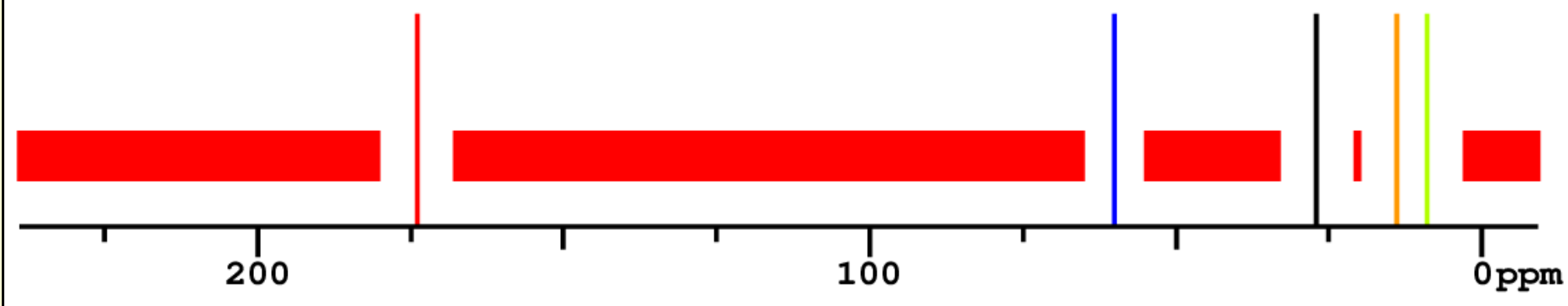
Predicted shift values

Signal multiplicity: S D T Q O E P ?



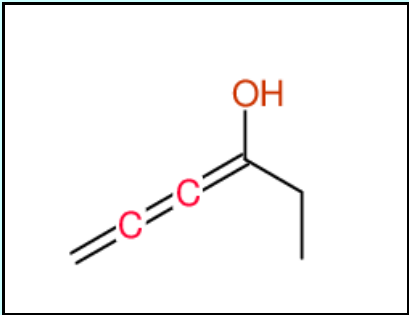
Experimental shift values

No line in reference: 

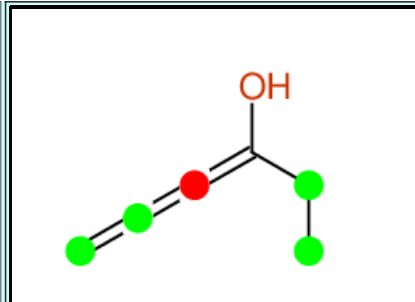
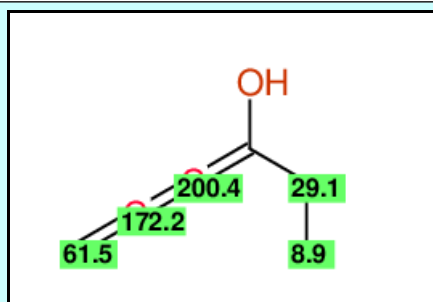


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### Structure Proposal #42

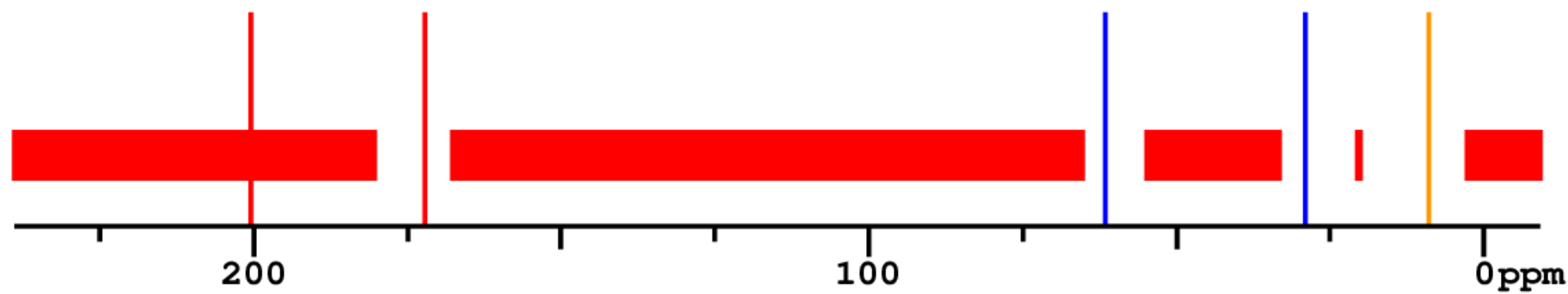
Structure	Similarity Measure
	<p>Deviation = 6.91 ppm Similarity = 80 % (Different pattern)</p> <p><math>C_6H_8O</math></p> <p>MWT = 96.07</p> <p>Search Web for this structure: <a href="#">XEXVNBAJTJGVQJ</a></p>
Predicted Chemical Shiftvalues	Matching Map





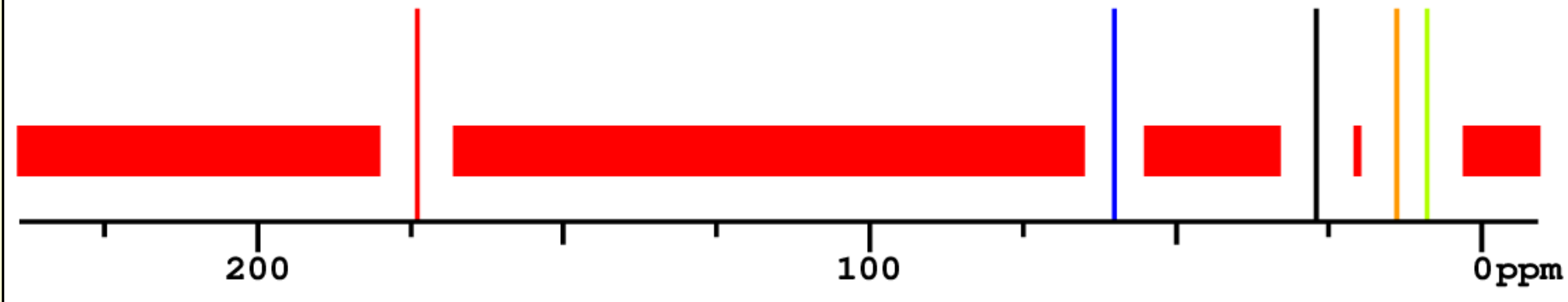
Predicted shift values

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



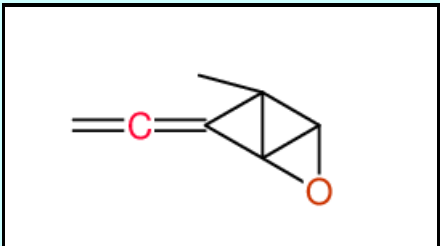
Experimental shift values

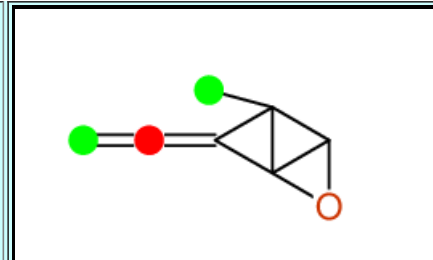
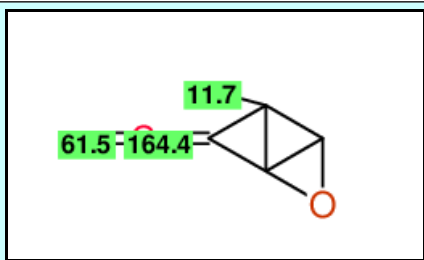
No line in reference: 



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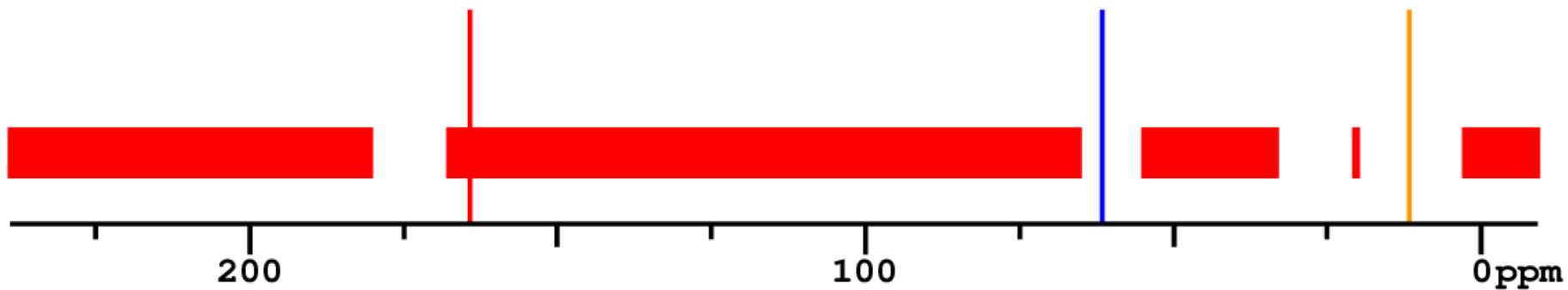
### Structure Proposal #43

Structure	Similarity Measure
	<p>Deviation = 7.38 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_7H_6O</math></p> <p>MWT = 106.08</p> <p>Search Web for this structure: <a href="#">JVINKFDAUHPDE</a></p>
Predicted Chemical Shiftvalues	Matching Map



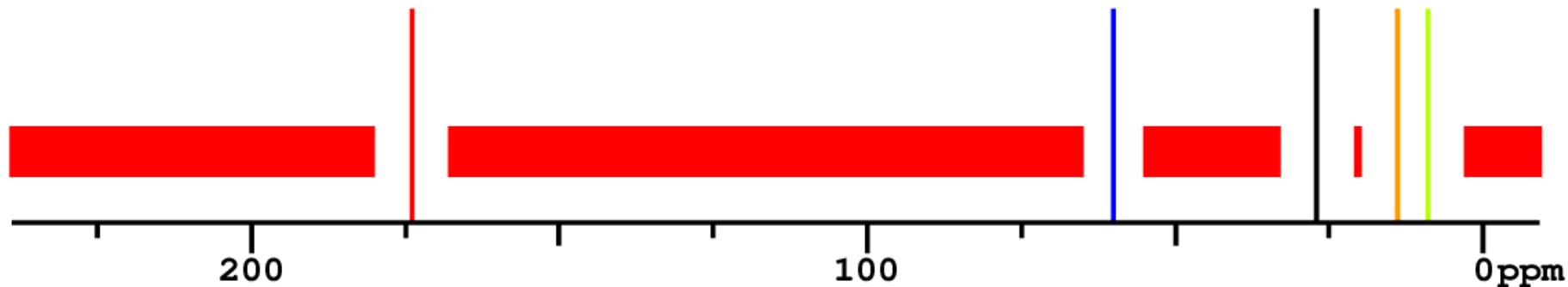
Predicted shift values

Signal multiplicity: S D T Q O E P ?



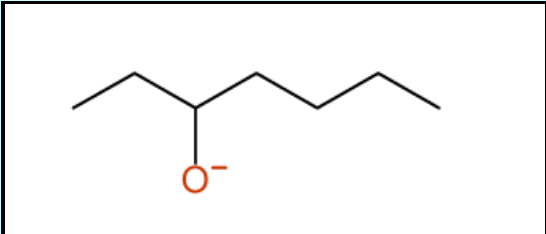
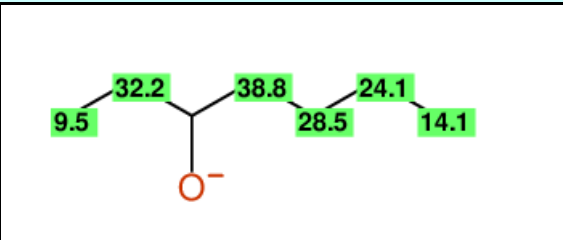
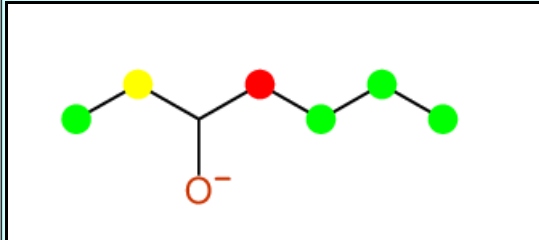
Experimental shift values

No line in reference: ████████



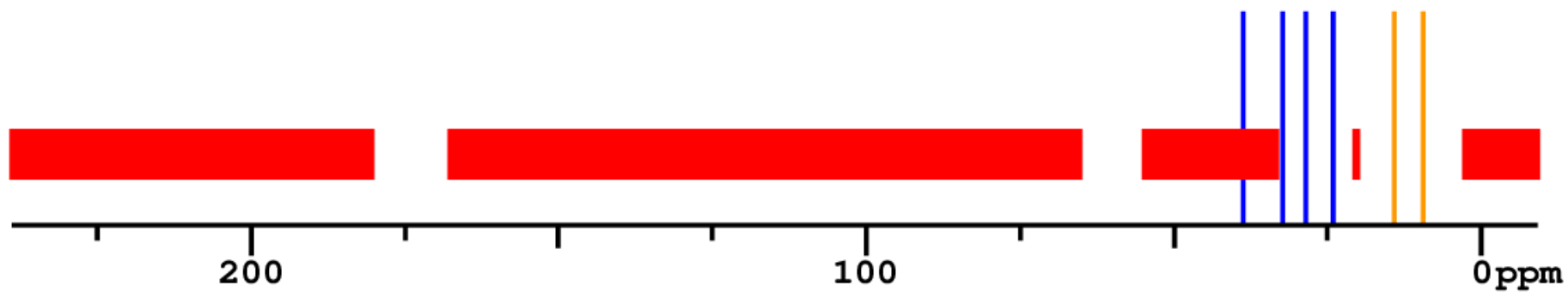
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### Structure Proposal #44

Structure	Similarity Measure
	<p>Deviation = 7.72 ppm Similarity = 75 % (Different pattern)</p> <p><math>C_7H_{15}O</math></p> <p>MWT = 115.08</p> <p>Search Web for this structure: <a href="#">ORSCOPLJPMQZHQ</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

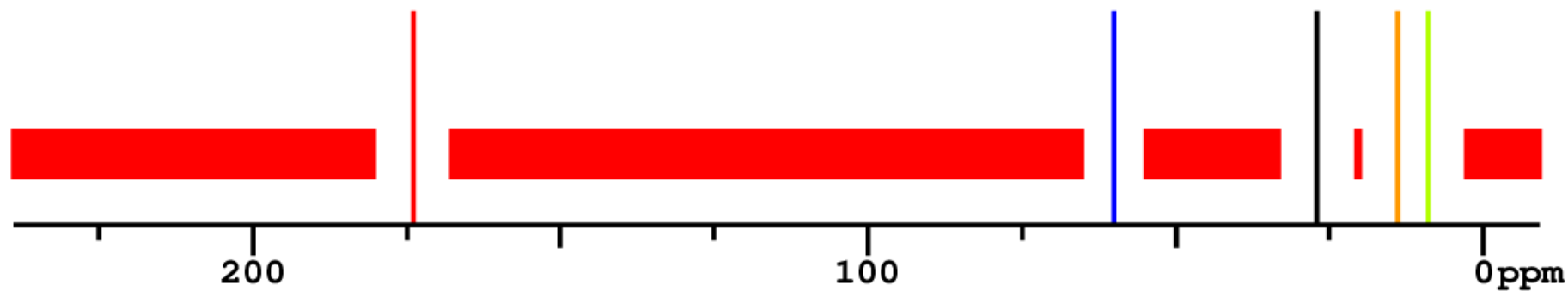
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

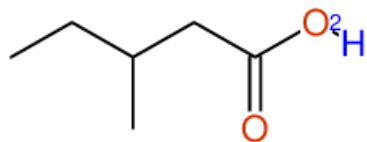
No line in reference: [red bar]



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### Structure Proposal #45

Structure	Similarity Measure



Deviation = 7.90 ppm  
 Similarity = 58 %  
 (Different pattern)

$C_6H_{12}O_2$

MWT = 117.07

Search Web for this structure:

[IGIDL TISMCAULB](#)

Predicted Chemical Shiftvalues

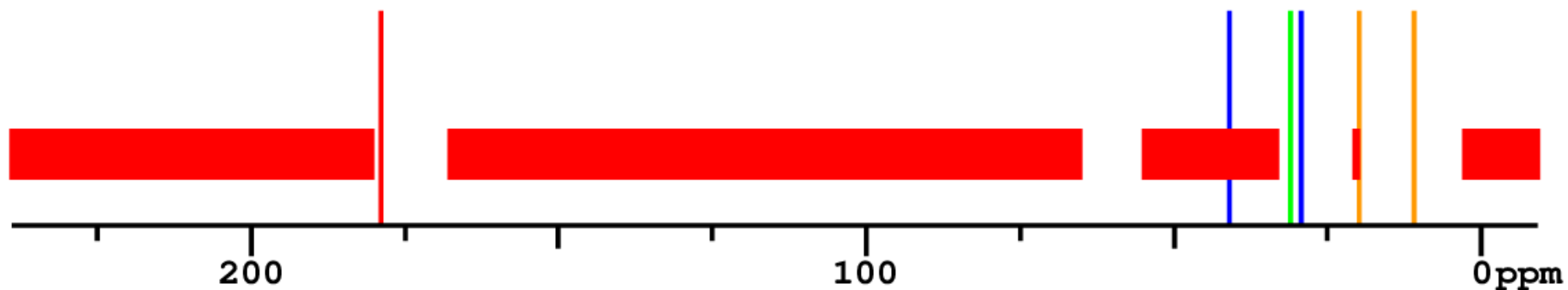


Matching Map



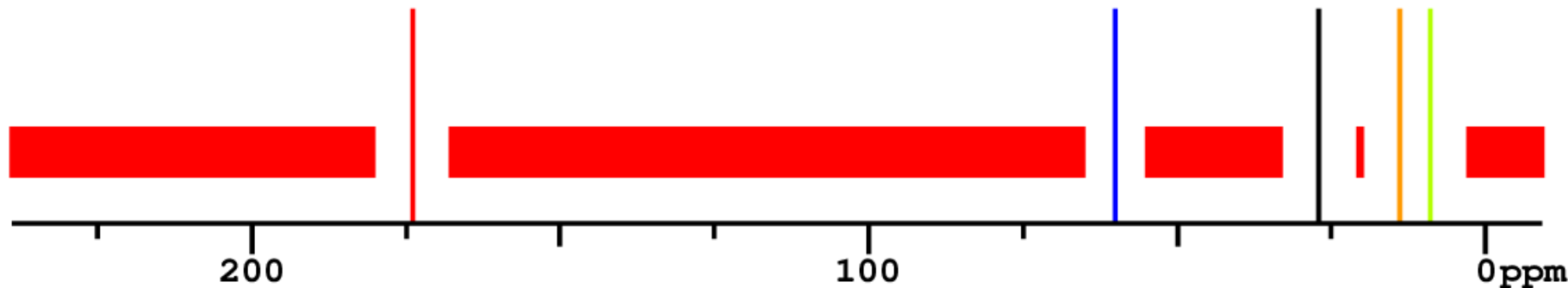
Predicted shift values

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



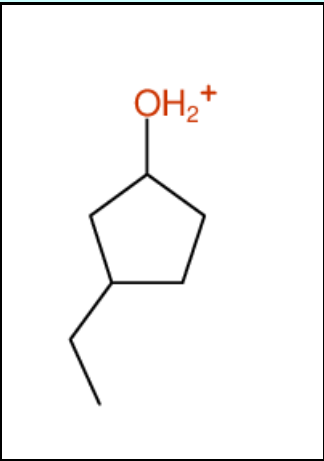
Experimental shift values

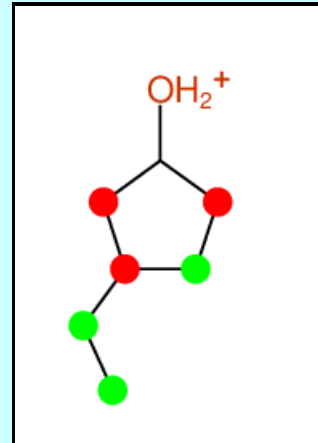
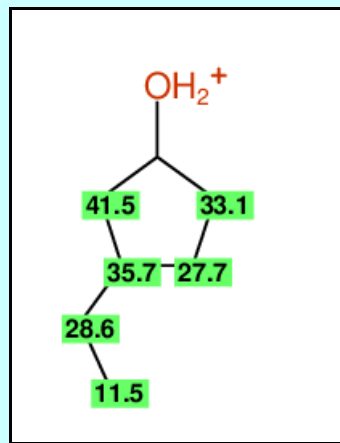
No line in reference: 



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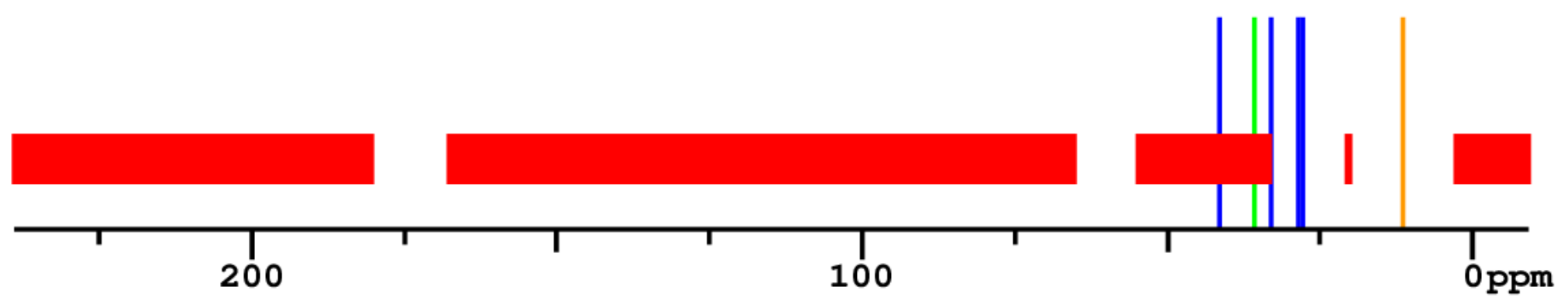
### Structure Proposal #46

Structure	Similarity Measure
	<p>Deviation = 8.04 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_7H_{14}O</math></p> <p>MWT = 114.08</p> <p>Search Web for this structure: <a href="#">CRHZGBUSTWVQAQ</a></p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

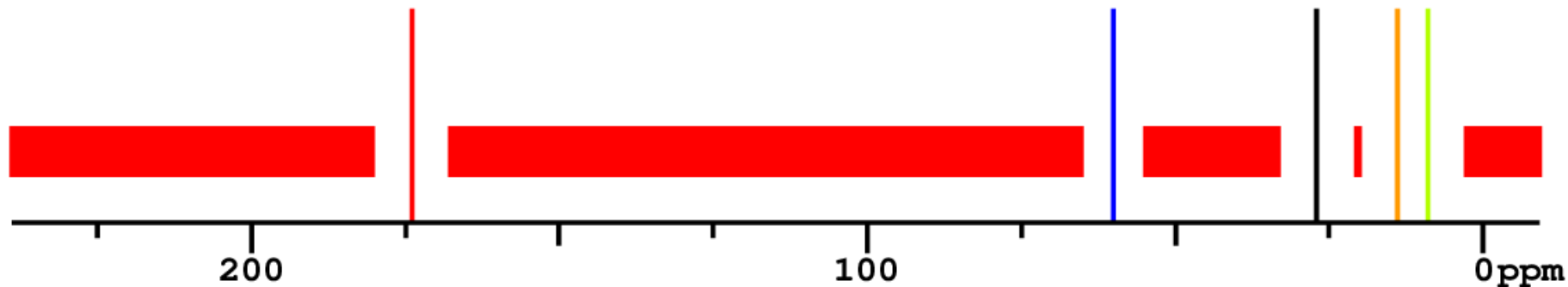
Signal multiplicity: S D T Q O E P ?





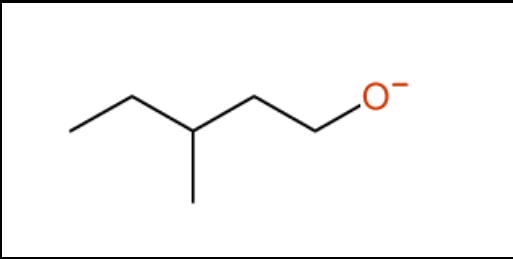
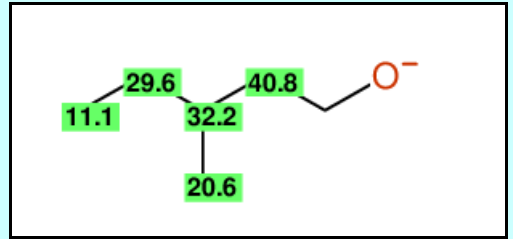
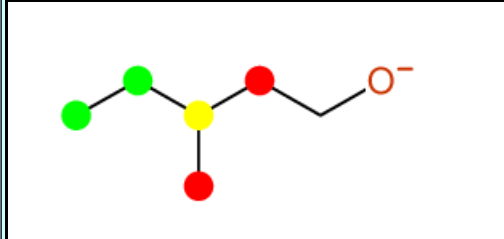
Experimental shift values

No line in reference: ████████



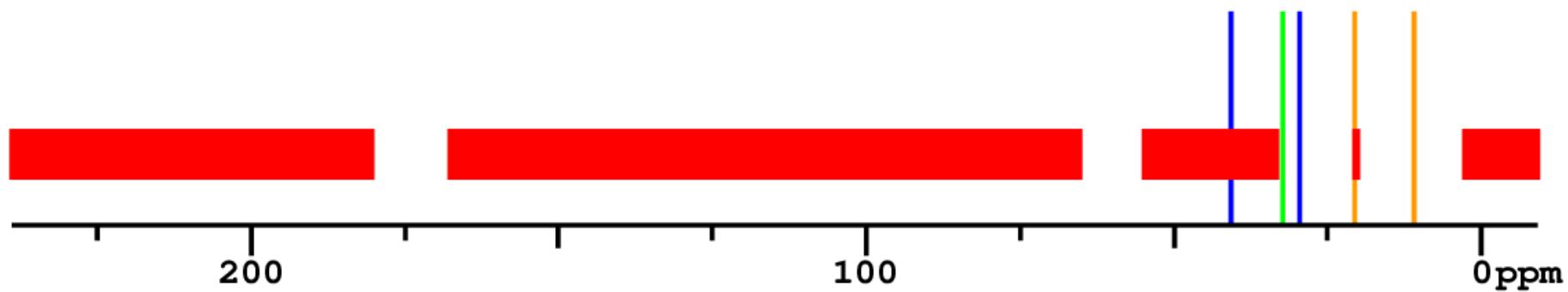
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### Structure Proposal #47

Structure	Similarity Measure
	<p>Deviation = 8.12 ppm Similarity = 50 % (Different pattern)</p> <p><math>C_6H_{13}O</math></p> <p>MWT = 101.07</p> <p>Search Web for this structure: <a href="#">PMTZOPAULJSVJK</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

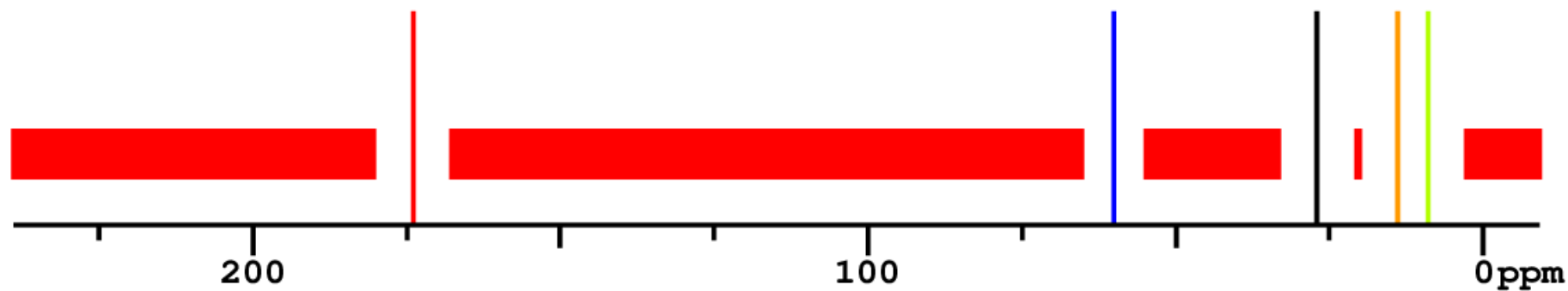
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

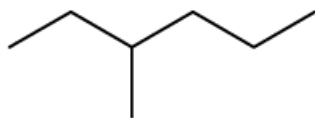
No line in reference: [red bar]



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### Structure Proposal #48

Structure	Similarity Measure



H<sub>2</sub>O

Deviation = 8.21 ppm

Similarity = 43 %

(Different pattern)

C<sub>7</sub>H<sub>16</sub>·H<sub>2</sub>O

MWT = 118.08

Search Web for this structure:

[GGYAZEDJULRYKQ](#)

Predicted Chemical Shiftvalues



H<sub>2</sub>O

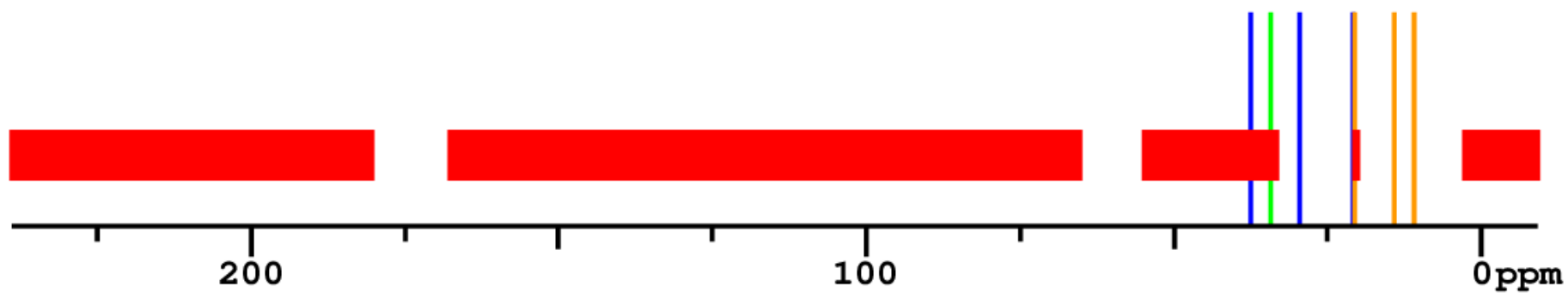
Matching Map



H<sub>2</sub>O

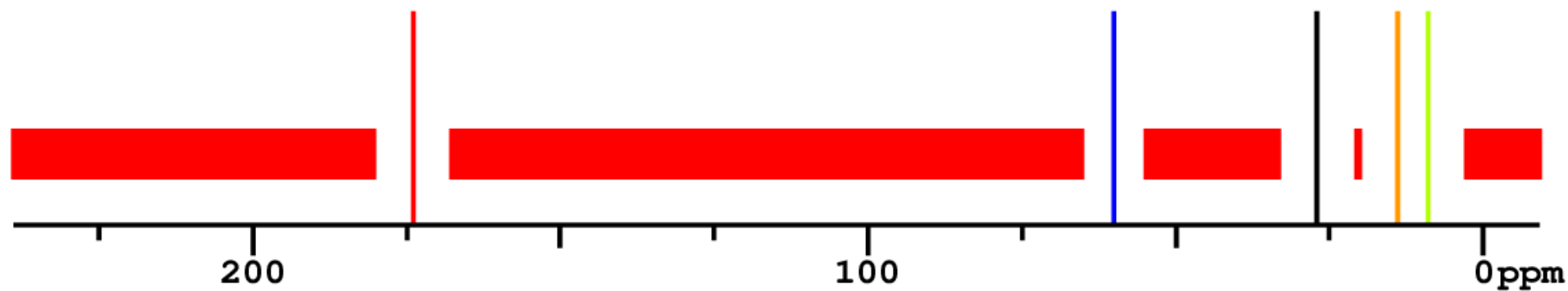
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

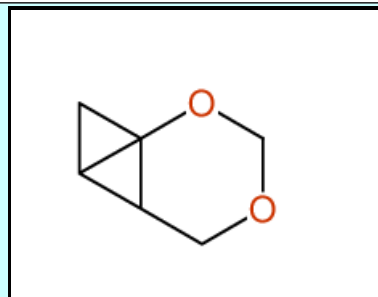
No line in reference: [red bar]



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### Structure Proposal #49

Structure	Similarity Measure
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Deviation = 8.39 ppm  
 Similarity = 75 %  
 (Different pattern)

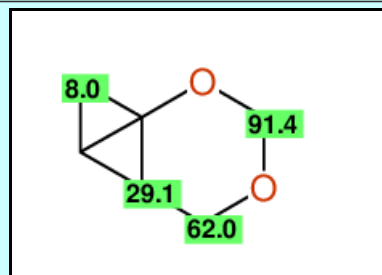


MWT = 112.07

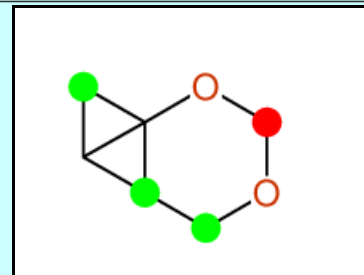
Search Web for this structure:

[VOOBIWANMYOOKZ](#)

Predicted Chemical Shiftvalues

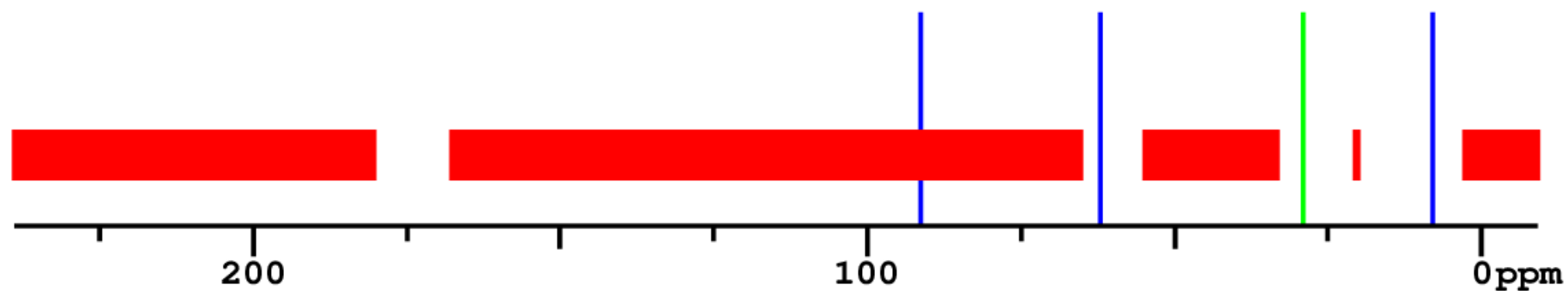


Matching Map



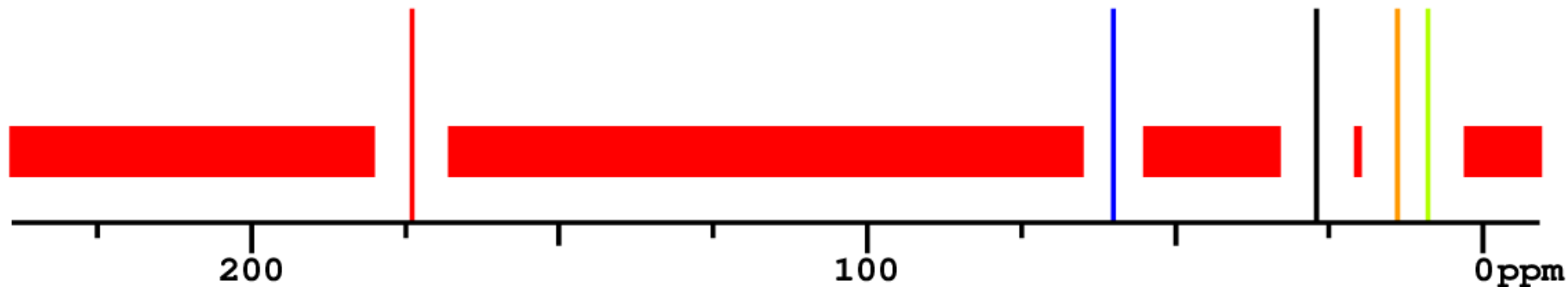
Predicted shift values

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



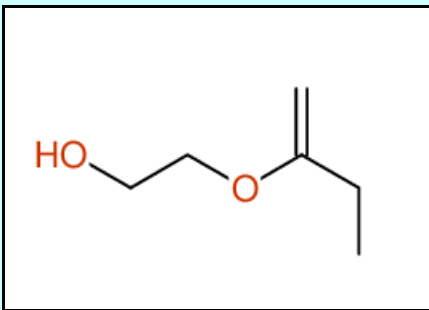
Experimental shift values

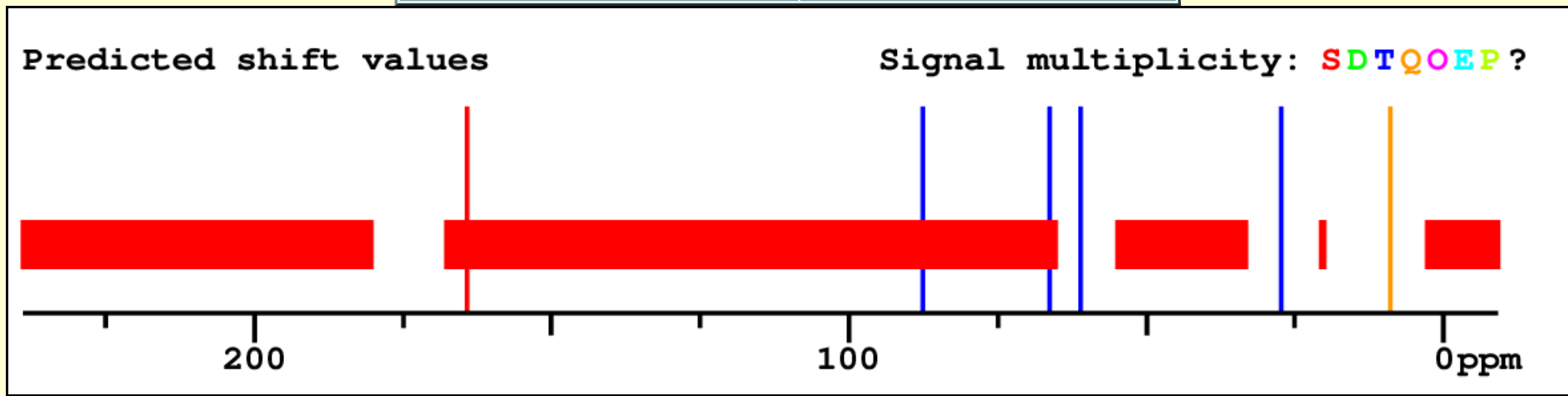
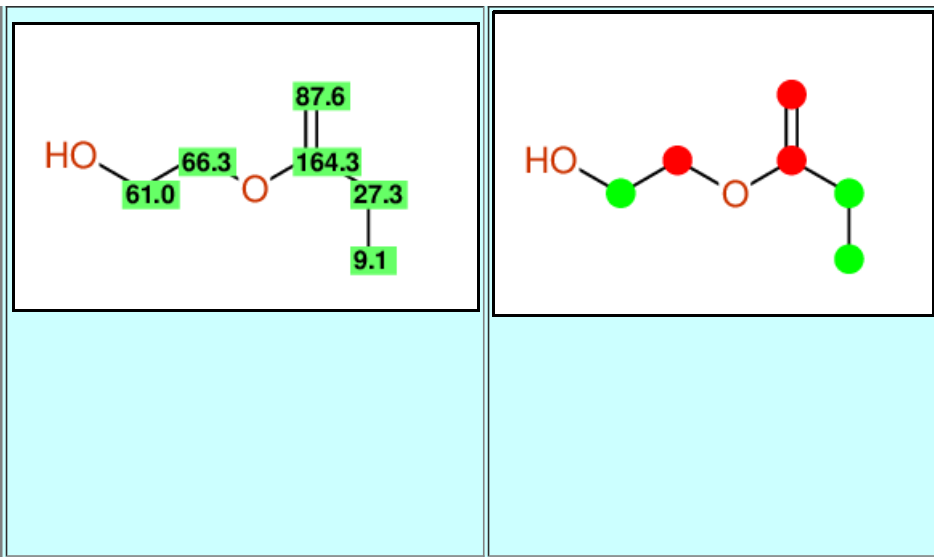
No line in reference: ████████



[Back to Complete Result](#)

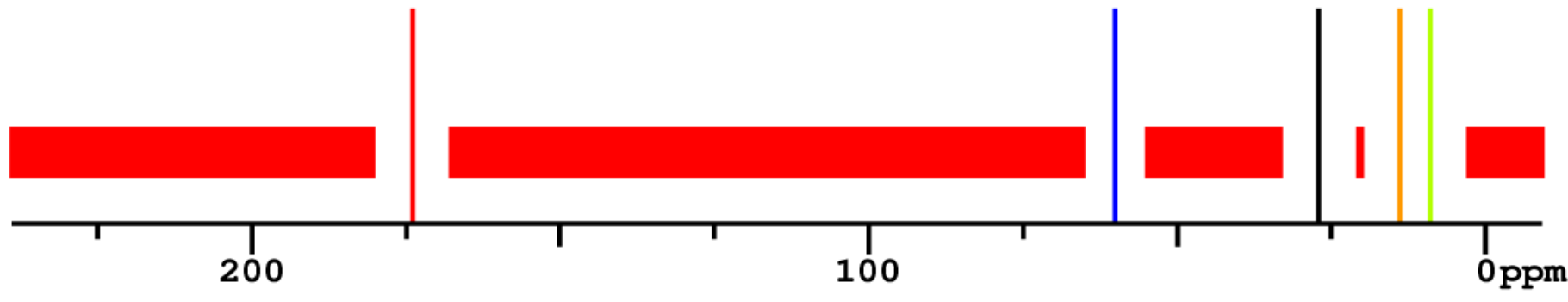
### Structure Proposal #50

Structure	Similarity Measure
	<p>Deviation = 8.56 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="#">XCNGAPQCDVGISX</a></p>
Predicted Chemical Shiftvalues	Matching Map



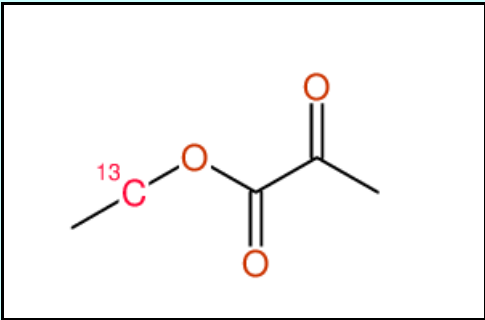
Experimental shift values

No line in reference: 

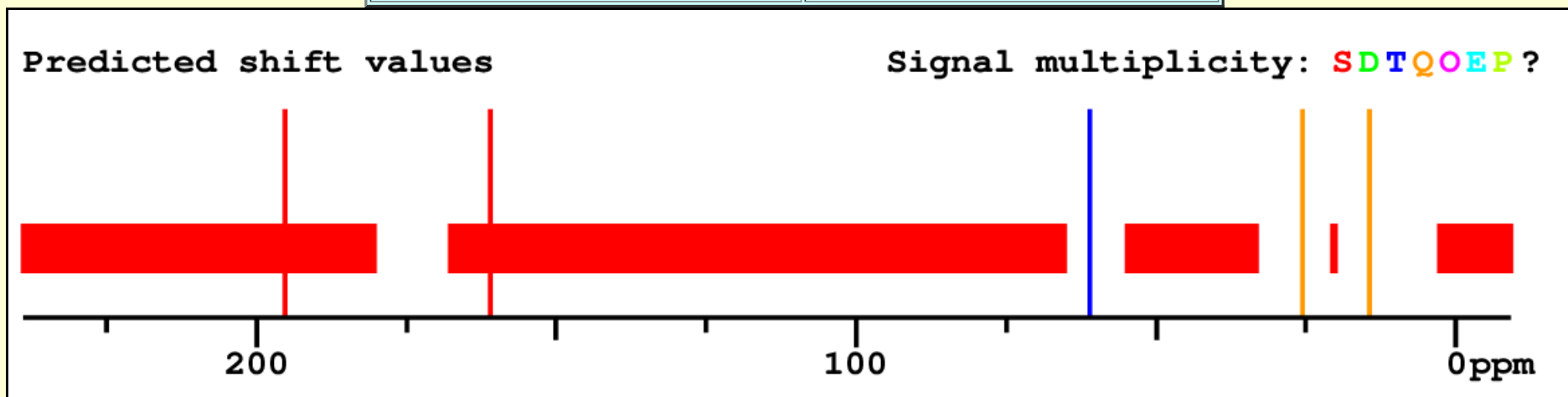
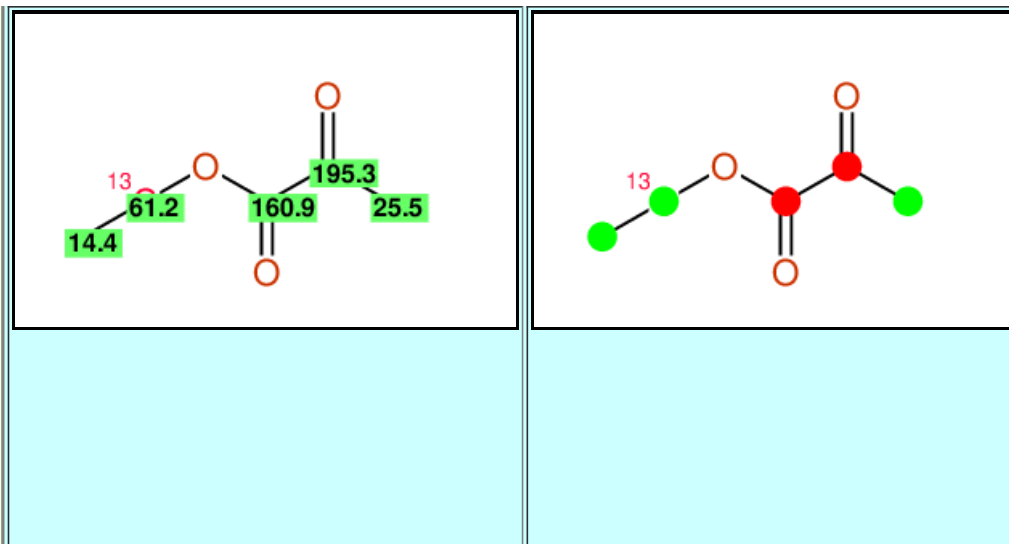


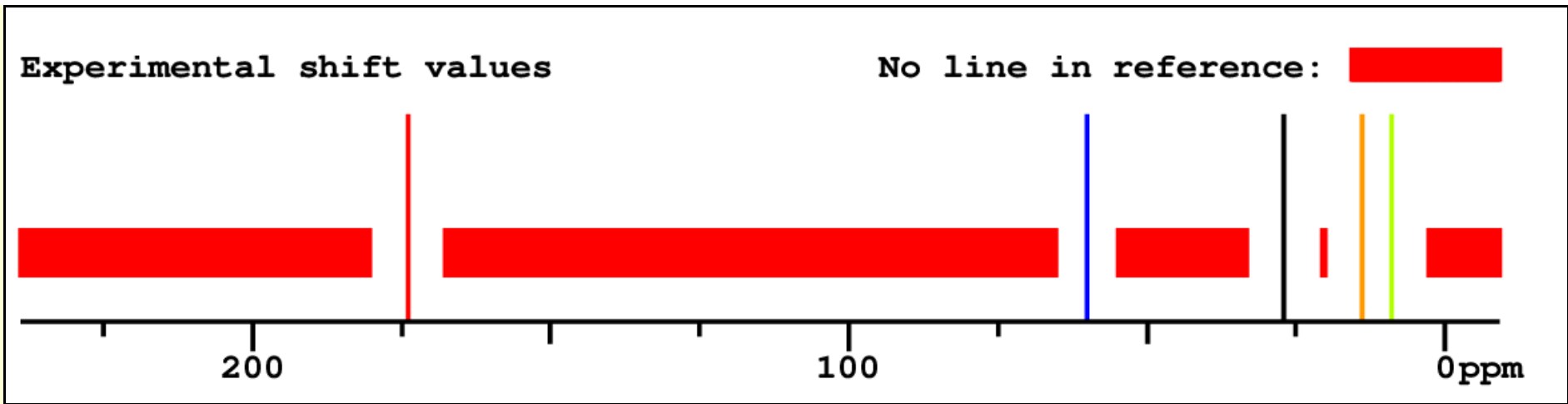
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### Structure Proposal #51

Structure	Similarity Measure
	<p>Deviation = 8.81 ppm Similarity = 60 % (Different pattern)</p> <p><math>C_5H_8O_3</math></p> <p>MWT = 117.06</p> <p>Search Web for this structure: <a href="#">XXRCUYYCPSWGCC</a> <a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map

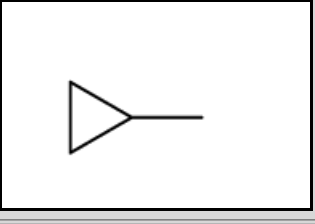
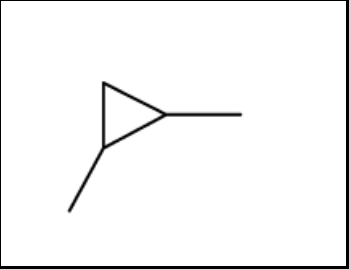






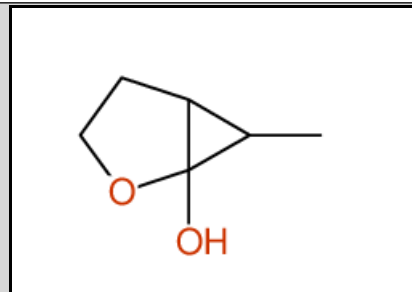
[Back to Complete Result](#)

**Summary of the 8 most frequently occurring parent ring systems  
within the 36 best-fitting entries**

<p>Occurrence: 2 in 36</p>			
<p>Occurrence: 1 in 36</p>			

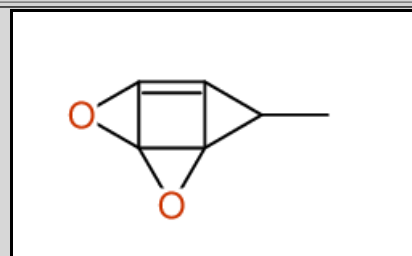
Occurrence:

1 in 36



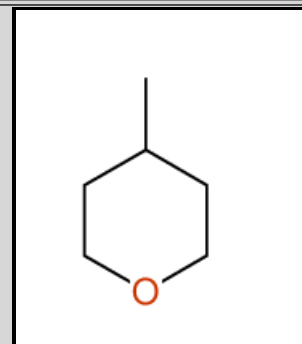
Occurrence:

1 in 36



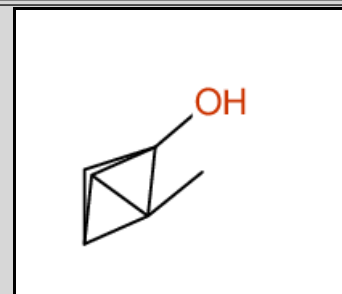
Occurrence:

1 in 36



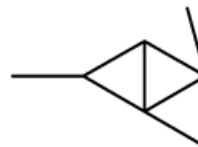
Occurrence:

1 in 36



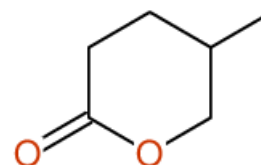
Occurrence:

1 in 36



Occurrence:

1 in 36



### Summary of Processing

Checking existence of data and counting them:	144,833,798 entries in 2.827 seconds
Applying restraints from elemental composition:	8.363 seconds, 3,593,931 entries remain
Applying restraints from number of signals:	3.710 seconds, 104,807 entries remain
Searching 2,390,716,602 chemical shift values line-per-line:	26.670 seconds
Best 4,653 entries selected for analysis:	3.204 seconds
Ranking of 4,653 entries by similarity:	212.643 seconds
Deviation of best match:	2.73 ppm
Creating table and linking 4,653 structures to 475,803 INCHIKEY-pages:	1.999 seconds
Detailed Analysis of 51 structures including graphical representation:	17.495 seconds
Analysis of 36 structures for common parent ring systems:	0.007 seconds
Total CPU-usage:	278.150 seconds

<b>Data transferred from disk:</b>	<b>1,676 MBytes out of 2,186,577 MBytes</b>
<b>Program version:</b>	<b>20200916_2-3D-zip/00</b>
<b>Machine:</b>	<b>I9-9900K / 16x3.60GHz</b>
<p><b>Page written by Wolfgang Robien using CSEARCH-Technology</b> <b>Page written on 2021:05:19 at 19:08</b> <b>Page finished on 2021:05:19 at 19:19</b></p> <p><b>Have a nice day !</b></p>	