

**Spectral Similarity Search based on
74,435,185 Structures from PUBCHEM using
CSEARCH - Technology**

Description of Request

Please cite this service as:

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

Automatic Resubmit:

Multiplicity omitted

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:08

This page will be kept for 30 days here

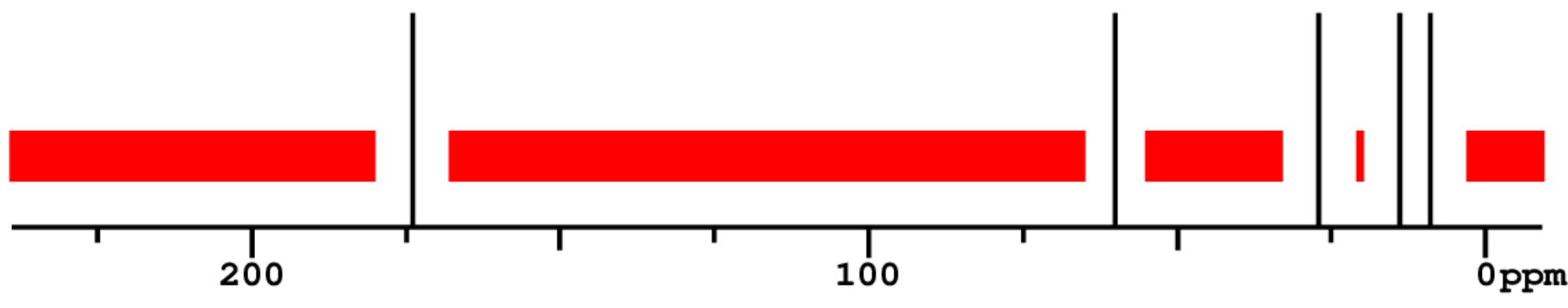
Name of Project:	Test1
Comment:	Dereplication-engine
Name of Compound:	Propionic_acid,ethylester 400MHz

Summary of Supplied Data

Peaklist given - consists of 5 Lines				
Line number	Chemical Shift (ppm)	Multiplicity	Hydrogens	Deviation (ppm)
1	174.00	?	C or CH or CH ₂ or CH ₃	3.00
2	60.00	?	C or CH or CH ₂ or CH ₃	2.50
3	27.00	?	C or CH or CH ₂ or CH ₃	3.00
4	14.00	?	C or CH or CH ₂ or CH ₃	3.00
5	9.00	?	C or CH or CH ₂ or CH ₃	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:	74,435,185
Compounds containing: N	67,903,871
Compounds containing: O	67,577,895
Compounds containing: P	930,048
Compounds containing: S	23,841,191
Compounds containing: F	13,496,062
Compounds containing: Cl	13,294,181
Compounds containing: Br	4,754,113
Compounds containing: I	705,469
Compounds containing: other	1,987,940

Available entries at each Screening-Step

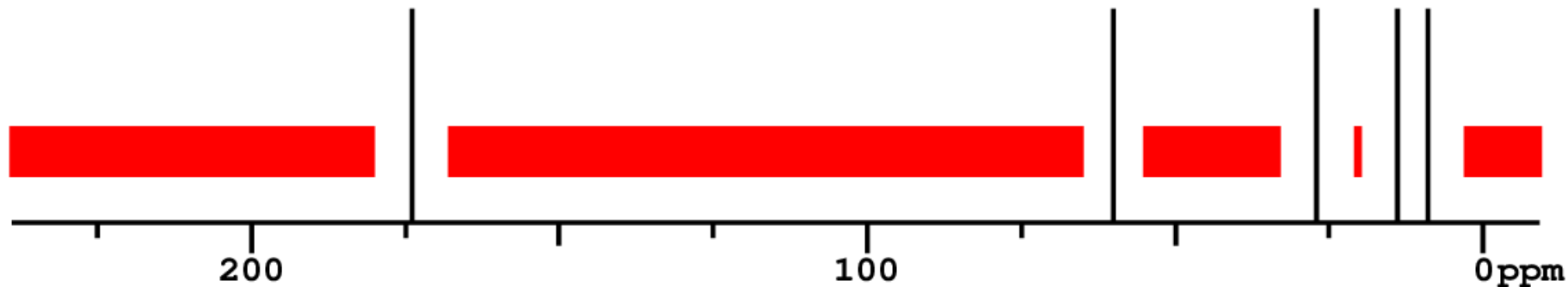
Total number of entries:	74,435,185
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Applying requested elemental composition:	2,773,229 entries remain
Applying requested number of signals:	170,467 entries remain

Entries per line found out of 170,467 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	?	3.00	30,069	Unspecific line
2	60.00	?	2.50	33,144	Unspecific line
3	27.00	?	3.00	66,806	Unspecific line
4	14.00	?	3.00	40,103	Unspecific line
5	9.00	?	3.00	21,657	Unspecific line

Experimental shift values

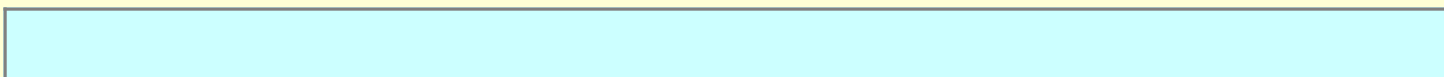
No line in reference: ██████████



Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	157	Selected for detailed analysis
4	1,843	Selected for detailed analysis
3	11,161	
2	39,071	
1	71,997	

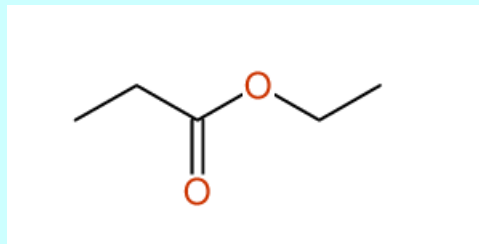
Best 18 Proposals shown for Compound: Propionic_acid,ethylester::400MHz



0.87 -
0.87ppm

3x found

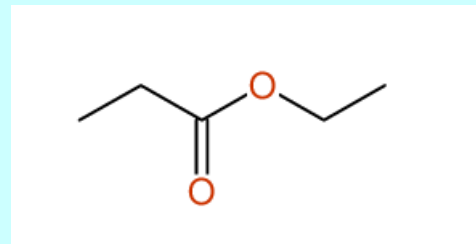
[FKRCODPIKNYEAC](#)



0.87 -
0.87ppm

1x found

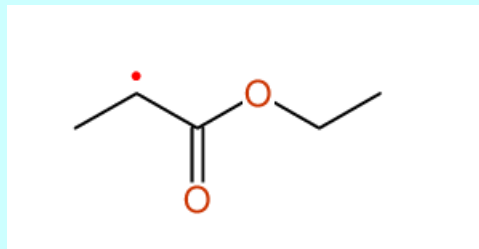
[BYLOWVUCDFUYIQ](#)



0.87 -
0.87ppm

1x found

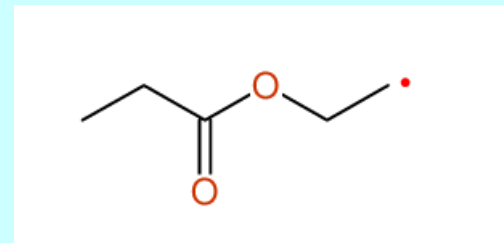
[UPLWNPAPKPC](#)



0.87 -
0.87ppm

1x found

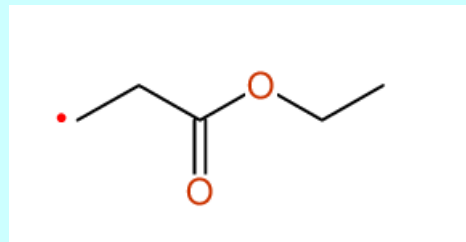
[IRGLFRDZYNBBCO](#)



0.87 -
0.87ppm

1x found

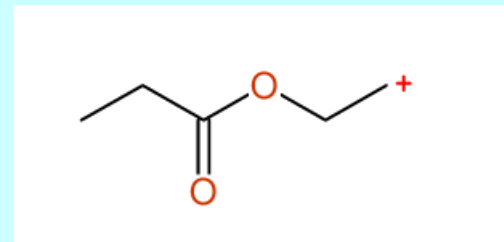
[SQKCNILPAQLIRC](#)



0.87 -
0.87ppm

1x found

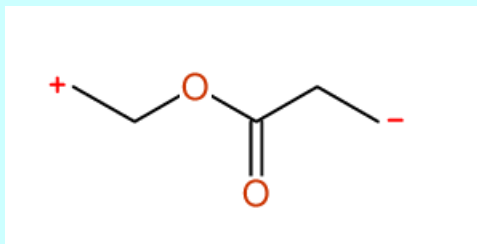
[GOKITYWXYBHPKU](#)



0.87 -
0.87ppm

1x found

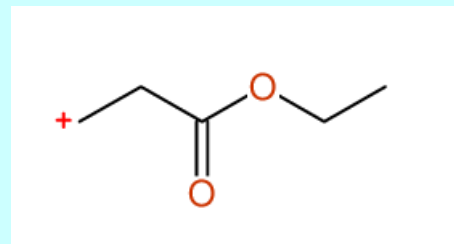
[LVCAAHDUTLIBML](#)



0.87 -
0.87ppm

1x found

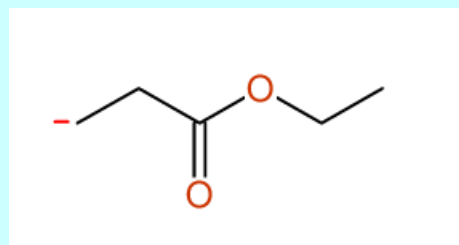
[MUQMZQYQIIBIT](#)



0.87 -
0.87ppm

1x found

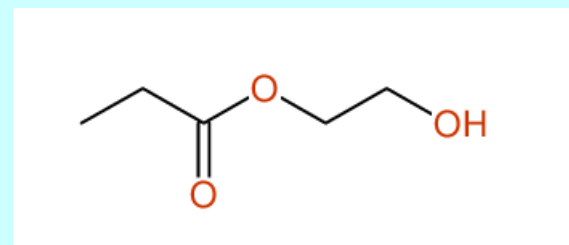
[NWIUUTFORIXPJC](#)



2.02 -
2.02ppm

1x found

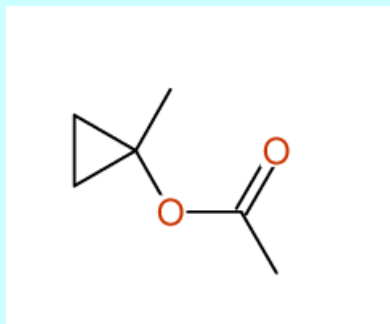
[SFAMKDPMPDEXGH](#)



2.45 -
2.45ppm

1x found

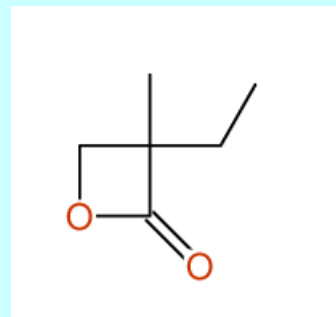
[MJRMRENBUDEGM](#)



4.17 -
4.17ppm

1x found

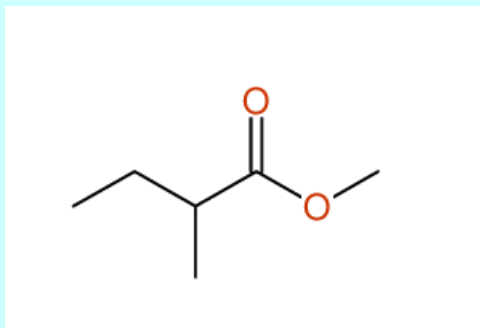
[UFTRVHTYHBMWOE](#)



5.25 -
5.25ppm

1x found

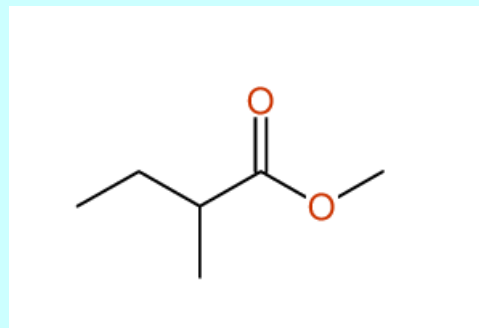
[YMRCZGBILKTSCL](#)

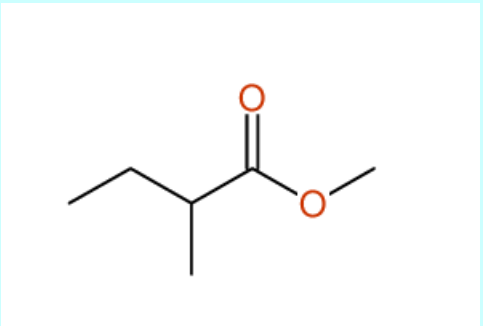
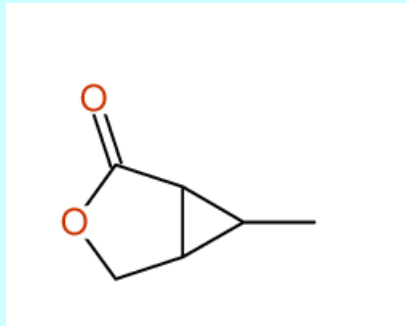
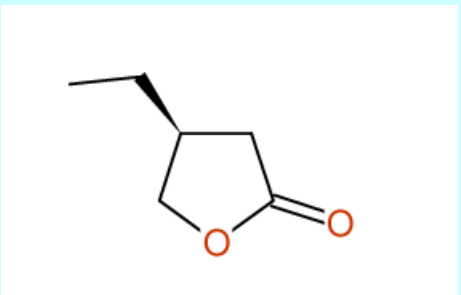
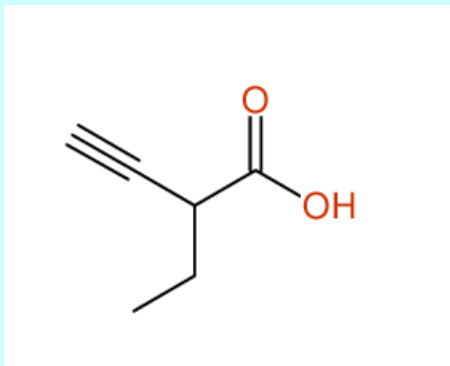


5.25 -
5.25ppm

1x found

[OYGDMLWOJBKWLN](#)

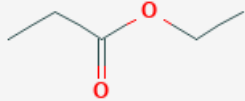

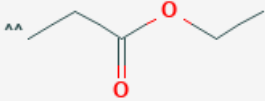


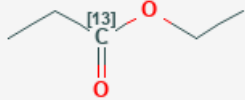

<p>5.25 - 5.25ppm 4x found OCWLYWIFNDCWRZ</p> 	<p>5.38 - 5.38ppm 1x found ODZSNSOKRZBPDY</p> 
<p>6.77 - 6.88ppm 2x found MDQZVJSUBKPTHG</p> 	<p>8.49 - 8.49ppm 1x found YHXLBJJLZTWBAZ</p> 

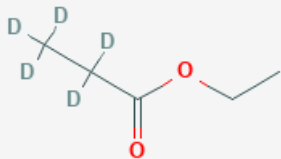

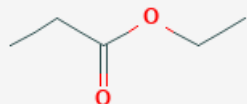
2,000 [Structure proposals](#) found for your C-NMR Spectrum

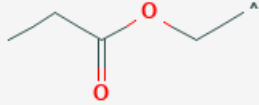
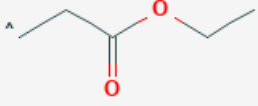
90 Entries will be shown because of your selection of additional constraints

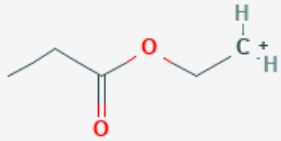
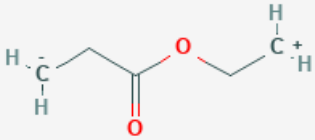
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
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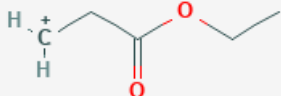
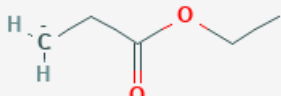
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 102.055</p>	<p>Proposal #1</p> <p>FKRCODPIKNYEAC-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 7749</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>0.87</p> <p>Details</p>		<p>$C_5H_8O_2$</p> <p>MWT = 100.055</p>	<p>Proposal #2</p> <p>BYLOWVUCDFUYIQ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 45120489</p>	

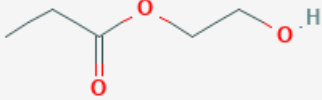
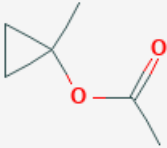
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details	 <p>The diagram shows the chemical structure of ethyl propyl ester. The carbonyl carbon is labeled with ¹³C. The ester group is shown as a carbonyl group (C=O) bonded to an ethyl group (CH₂CH₃) and an oxygen atom, which is further bonded to a propyl group (CH₂CH₂CH₃).</p>	C ₅ H ₁₀ O ₂ MWT = 103.055	Proposal #3 FKRCODPIKNYEAC-HOSYLAQJSA-N PUBCHEM Compound: 12229103	Availability of NMR-Data in CSEARCH 

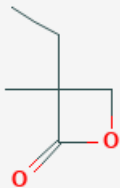
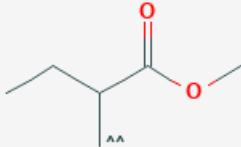
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>	 <p>The structure shows an acetate group with four deuterium atoms (D) attached to the methyl carbon and the alpha carbon. The ester oxygen is connected to an ethyl group.</p>	<p>$C_5H_{10}O_2$</p> <p>MWT = 107.055</p>	<p>Proposal #4</p> <p>FKRCODPIKNYEAC-WNWXXORZSA-N</p> <p>PUBCHEM Compound: 89254459</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>0.87</p> <p>Details</p>	 <p>The structure shows a standard acetate group with an ethyl group attached to the ester oxygen.</p>	<p>$C_5H_9O_2$</p> <p>MWT = 101.055</p>	<p>Proposal #5</p> <p>UPRLWNPAOPKPCE-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 5371171</p>	

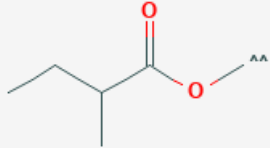
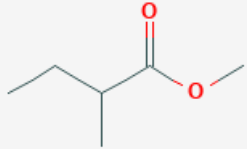

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details	 <p>Chemical structure diagram of ethyl propanoate, showing a propanoate group (CH₃CH₂COO-) and an ethyl group (-CH₂CH₃) attached to the oxygen atom.</p>	C ₅ H ₉ O ₂ MWT = 101.055	Proposal #6 IRGLFRDZYNBBCO-UHFFFAOYSA-N PUBCHEM Compound: 57419189	
0.87 Details	 <p>Chemical structure diagram of propyl propanoate, showing a propanoate group (CH₃CH₂COO-) and a propyl group (-CH₂CH₂CH₃) attached to the oxygen atom.</p>	C ₅ H ₉ O ₂ MWT = 101.055	Proposal #7 SQKCNILPAQLIRC-UHFFFAOYSA-N PUBCHEM Compound: 12568583	

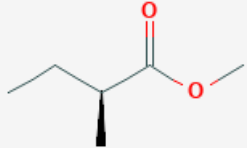

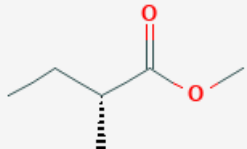

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_9O_2^+$</p> <p>MWT = 101.055</p>	<p>Proposal #8</p> <p>GOKITYWXYBHPKU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57582310</p>	
<p>0.87</p> <p>Details</p>		<p>$C_5H_8O_2$</p> <p>MWT = 100.055</p>	<p>Proposal #9</p> <p>LVCAAHDUTLIBML-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 53630283</p>	

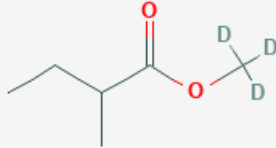

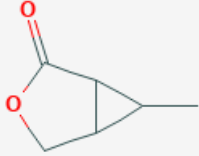
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_9O_2^+$</p> <p>MWT = 101.055</p>	<p>Proposal #10</p> <p>MUQMZQYQIIZBIT-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 91194346</p>	
<p>0.87</p> <p>Details</p>		<p>$C_5H_9O_2^-$</p> <p>MWT = 101.055</p>	<p>Proposal #11</p> <p>NWIUUTFORIXPJC-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 91508541</p>	

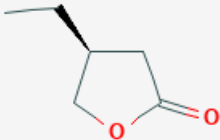

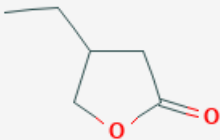

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>2.02</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 118.055</p>	<p>Proposal #12</p> <p>SFAMKDPMPDEXGH-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 545098</p>	
<p>2.45</p> <p>Details</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #13</p> <p>MJRMRENBUDEGM-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 2735228</p>	

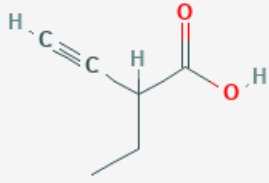
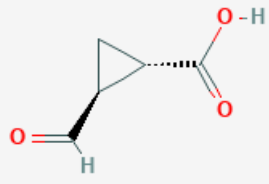
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>4.17</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #14</p> <p>UFTRVHTYHBMWOF-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 14318253</p>	
<p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #15</p> <p>YMRCZGBILKTSCSCL-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 59258212</p>	

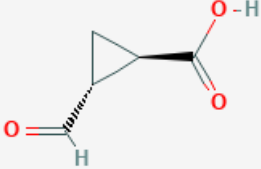
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #16</p> <p>OYGDMLWOJBKWLN-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 59990131</p>	
<p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #17</p> <p>OCWLYWIFENDCWRZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 13357</p>	<p>Availability of NMR-Data in CSEARCH</p> 

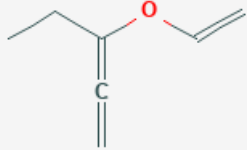

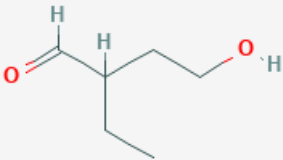
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #18</p> <p>OCWLYWIFNDCWRZ-YFKPBYRVSA-N</p> <p>PUBCHEM Compound: 643001</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #19</p> <p>OCWLYWIFNDCWRZ-RXMQYKEDSA-N</p> <p>PUBCHEM Compound: 644216</p>	<p>Availability of NMR-Data in CSEARCH</p> 

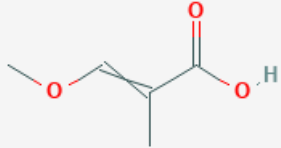
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>5.25</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a four-carbon chain with a methyl group on the second carbon and a carboxylic acid group on the first carbon. The four alpha-hydrogens (on the second, third, and fourth carbons) are replaced by deuterium atoms (D).</p>	<p>$C_6H_{12}O_2$</p> <p>MWT = 119.066</p>	<p>Proposal #20</p> <p>OCWLYWIFNDCWRZ-HPRDVNIFSA-N</p> <p>PUBCHEM Compound: 60069722</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>5.38</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a three-membered cyclopropane ring with a methyl group and a carboxylic acid group attached to one of the ring carbons.</p>	<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #21</p> <p>ODZSNSOKRZBPDY-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 11228776</p>	

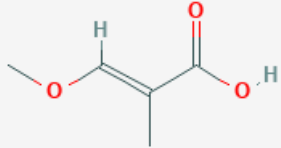
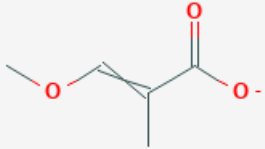
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>6.77</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #22</p> <p>MDQZVJSUBKPTHG-YFKPBYRVSA-N</p> <p>PUBCHEM Compound: 57939696</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>6.88</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #23</p> <p>MDQZVJSUBKPTHG-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 27893</p>	<p>Availability of NMR-Data in CSEARCH</p> 

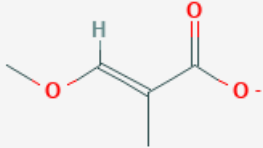

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>8.49</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #24</p> <p>YHXLBJJLZTWBAZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12491392</p>	
<p>13.89</p> <p>Different pattern</p>		<p>$C_5H_6O_3$</p> <p>MWT = 114.055</p>	<p>Proposal #25</p> <p>VOVAKSXCTQYGIH-DMTCNVIQSA-N</p> <p>PUBCHEM Compound: 89189889</p>	

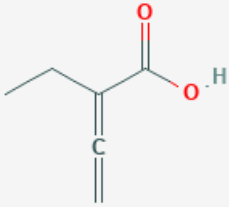
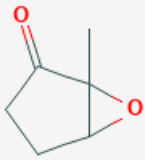
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>13.89</p> <p>Different pattern</p>	 <p>The structure shows a cyclopropyl ring with a carboxylic acid group (-COOH) attached to one carbon and an aldehyde group (-CHO) attached to an adjacent carbon. The aldehyde group is shown with a dashed bond to the ring, and the carboxylic acid group is shown with a wedged bond to the ring.</p>	<p>$C_5H_6O_3$</p> <p>MWT = 114.055</p>	<p>Proposal #26</p> <p>VOVAKSXCTQYGIH-IUYQGCFVSA-N</p> <p>PUBCHEM Compound: 55303491</p>	

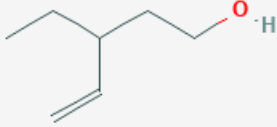
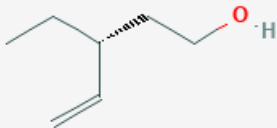
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>13.93</p> <p>Different pattern</p>		<p>$C_7H_{10}O$</p> <p>MWT = 110.077</p>	<p>Proposal #27</p> <p>MFKQNKFYXTLMB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 15084427</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>14.56</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #28</p> <p>CBSYYWQEKMTXTJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12367599</p>	

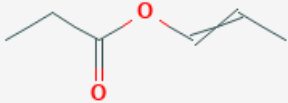
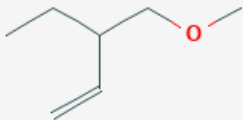
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
14.81 Different pattern	 <p>The structure diagram shows 3-methoxybutanoic acid. It consists of a four-carbon chain. The first carbon is part of a carboxylic acid group (COOH). The second carbon has a methyl group attached. The third carbon has a methoxy group (-OCH3) attached. The fourth carbon is a methyl group.</p>	C ₅ H ₈ O ₃ MWT = 116.055	Proposal #29 JQEBZBUGQPSANC-UHFFFAOYSA-N PUBCHEM Compound: 268572	

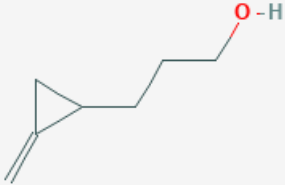

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>14.81</p> <p>Different pattern</p>	 <p>Chemical structure of methyl acrylate: <chem>C=CC(=O)OC</chem></p>	<p>$C_5H_8O_3$</p> <p>MWT = 116.055</p>	<p>Proposal #30</p> <p>JQEBZBUGQPSANC-ONEGZZNKSA-N</p> <p>PUBCHEM Compound: 5381014</p>	
<p>14.81</p> <p>Different pattern</p>	 <p>Chemical structure of methyl acrylate anion: <chem>C=CC(=O)[O-]OC</chem></p>	<p>$C_5H_7O_3^-$</p> <p>MWT = 115.055</p>	<p>Proposal #31</p> <p>JQEBZBUGQPSANC-UHFFFAOYSA-M</p> <p>PUBCHEM Compound: 53442773</p>	



Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>14.81</p> <p>Different pattern</p>		<p>$C_5H_7O_3^-$</p> <p>MWT = 115.055</p>	<p>Proposal #32</p> <p>JOEBZBUGOPSANC-ONEGZZNKSA-M</p> <p>PUBCHEM Compound: 86648308</p>	
<p>15.10</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #33</p> <p>CASOXAYOCHCWQU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 22558530</p>	

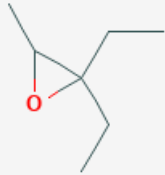

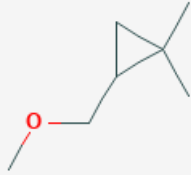
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>16.48</p> <p>Different pattern</p>	 <p>The structure shows a carboxylic acid group (COOH) attached to a carbon atom that is also part of a double bond. This carbon is further substituted with a methyl group and an ethyl group.</p>	<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #34</p> <p>PSBUQOAVEMYGEF-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 15570377</p>	
<p>18.21</p> <p>Different pattern</p>	 <p>The structure shows a five-membered ring with a ketone group (=O) and a methyl group attached to the same carbon atom.</p>	<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #35</p> <p>QQXRKGCBOXGHLK-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 85518914</p>	

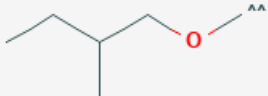
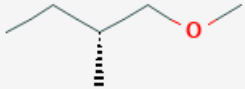
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>19.00</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #36</p> <p>LRKICXFRWQFSZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 86167614</p>	
<p>19.00</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #37</p> <p>LRKICXFRWQFSZ-SSDOTTWSA-N</p> <p>PUBCHEM Compound: 24767552</p>	

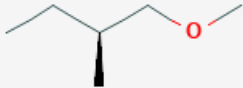
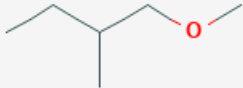
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>19.58</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #38</p> <p>AOJIRGQJECGWRU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 53653613</p>	
<p>19.87</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #39</p> <p>KNSUQQKLXTYXIY-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 54004268</p>	

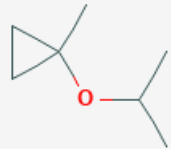
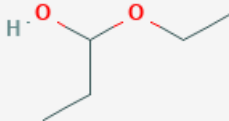

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>21.54</p> <p>Different pattern</p>		<p>$C_7H_{12}O$</p> <p>MWT = 112.077</p>	<p>Proposal #40</p> <p>UZKBINWCPUCLNB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 14940678</p>	
<p>25.38</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #41</p> <p>KFRVYYGHSPLXSZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 13527</p>	

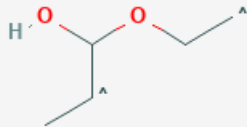
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.38</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 119.077</p>	<p>Proposal #42</p> <p>KFRVYYGHSPLXSZ-FIBGUPNXSA-N</p> <p>PUBCHEM Compound: 10534657</p>	
<p>25.38</p> <p>Different pattern</p>		<p>$C_7H_{15}O$</p> <p>MWT = 115.077</p>	<p>Proposal #43</p> <p>NFHQDZUNLMHWRI-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57481895</p>	

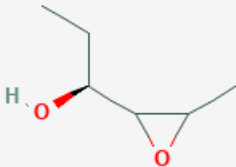
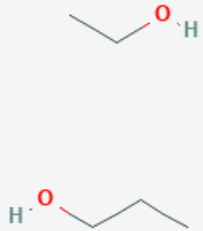
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
25.39		<p>C₇H₁₄O</p> <p>MWT = 114.077</p>	<p>Proposal #44</p> <p>BEBFQDLORXWCFR-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12936855</p>	<p>Availability of NMR-Data in CSEARCH</p> 
25.44 Different pattern		<p>C₇H₁₄O</p> <p>MWT = 114.077</p>	<p>Proposal #45</p> <p>JBMOKWDQRGLVSY-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 53682321</p>	

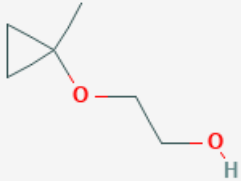
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.51</p> <p>Different pattern</p>		<p>$C_6H_{12}O$</p> <p>MWT = 100.066</p>	<p>Proposal #46</p> <p>MTIROVVXMQNOSL-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 58104734</p>	
<p>25.51</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #47</p> <p>XGLHRCWEOMNVKS-ZCFIWIBFSA-N</p> <p>PUBCHEM Compound: 54468195</p>	

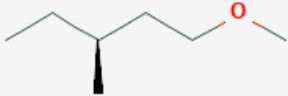
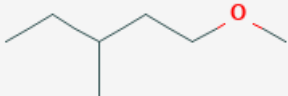
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.51</p> <p>Different pattern</p>		<p>C₆H₁₄O</p> <p>MWT = 102.066</p>	<p>Proposal #48</p> <p>XGLHRCWEOMNVKS-LURJTMIESA-N</p> <p>PUBCHEM Compound: 59954514</p>	
<p>25.51</p> <p>Different pattern</p>		<p>C₆H₁₄O</p> <p>MWT = 102.066</p>	<p>Proposal #49</p> <p>XGLHRCWEOMNVKS-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 522007</p>	

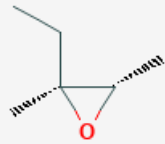

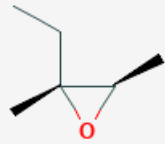

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.56</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #50</p> <p>TYDALWAMLXJDBB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 20782632</p>	
<p>25.56</p> <p>Different pattern</p>		<p>$C_5H_{12}O_2$</p> <p>MWT = 104.055</p>	<p>Proposal #51</p> <p>JLBXCKSMESLGTJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 93269</p>	<p>Availability of NMR-Data in CSEARCH</p> 

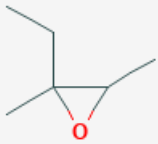


Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.56</p> <p>Different pattern</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 102.055</p>	<p>Proposal #52</p> <p>VOZYDHLZQKQCB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 90787265</p>	

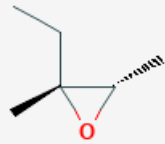

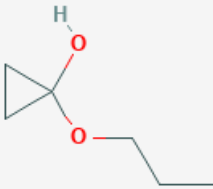
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>25.73</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #53</p> <p>MADOEHZKQDEEDD-XRVVJQKQSA-N</p> <p>PUBCHEM Compound: 11073387</p>	
<p>25.83</p>		<p>$C_5H_{14}O_2$</p> <p>MWT = 106.055</p>	<p>Proposal #54</p> <p>OMRDZQXXMYCHBU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 9793718</p>	

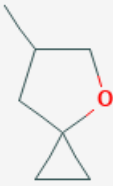
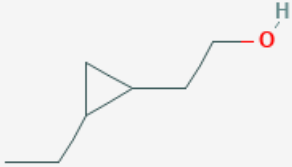

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
25.92 Different pattern		C ₆ H ₁₂ O ₂ MWT = 116.066	Proposal #55 TYIFOPYCGBVBFC-UHFFFAOYSA-N PUBCHEM Compound: 59557732	

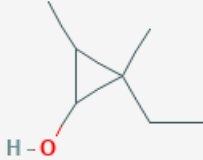


Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>26.22</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #56</p> <p>NRRLQGHHRCTIAS-ZETCQYMHSA-N</p> <p>PUBCHEM Compound: 59708443</p>	
<p>26.22</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #57</p> <p>NRRLQGHHRCTIAS-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 15706803</p>	

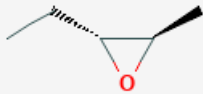



Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
26.39		<p>$C_6H_{12}O$ MWT = 100.066</p>	<p>Proposal #58 ZISUZIXPPXXNPC-WDSKDSINSA-N PUBCHEM Compound: 11804685</p>	<p>Availability of NMR-Data in CSEARCH</p> 
26.39		<p>$C_6H_{12}O$ MWT = 100.066</p>	<p>Proposal #59 ZISUZIXPPXXNPC-PHDIDXHHSA-N PUBCHEM Compound: 91567965</p>	<p>Availability of NMR-Data in CSEARCH</p> 

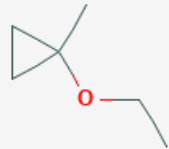
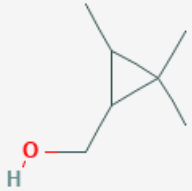
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
26.45		$C_6H_{12}O$ MWT = 100.066	Proposal #60 ZISUZIXPPXXNPC-UHFFFAOYSA-N PUBCHEM Compound: 12936856	Availability of NMR-Data in CSEARCH 
26.52		$C_7H_{18}O$ MWT = 118.077	Proposal #61 ZARMDFHSJSIZKQ-UHFFFAOYSA-N PUBCHEM Compound: 54537300	


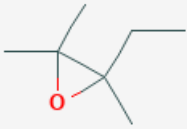
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>26.56</p> <p>Different pattern</p>		<p>$C_6H_{12}O$</p> <p>MWT = 100.066</p>	<p>Proposal #62</p> <p>ZISUZIXPPXXNPC-NTSWFWBYSA-N</p> <p>PUBCHEM Compound: 59911370</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>26.75</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #63</p> <p>MVQNTTWSJWGYBW-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 91475126</p>	

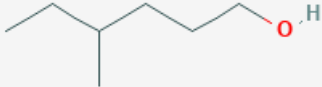

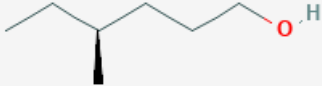

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>26.78</p> <p>Different pattern</p>		<p>$C_7H_{12}O$</p> <p>MWT = 112.077</p>	<p>Proposal #64</p> <p>BGRNLZJZEUFWIV-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 90127780</p>	
<p>26.78</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #65</p> <p>IPKMDCPNAOYUEB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 23329956</p>	<p>Availability of NMR-Data in CSEARCH</p> 

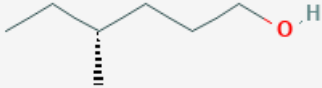

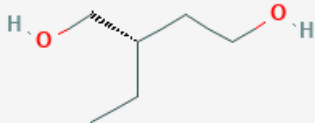
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
26.84		<p>$C_7H_{14}O$ MWT = 114.077</p>	<p>Proposal #66 AGOYXRWCLUIGIT-UHFFFAOYSA-N PUBCHEM Compound: 91532137</p>	
26.92		<p>$C_5H_{10}O$ MWT = 86.055</p>	<p>Proposal #67 BCJPEZMFAKOJPM-UHFFFAOYSA-N PUBCHEM Compound: 520554</p>	<p>Availability of NMR-Data in CSEARCH</p> 

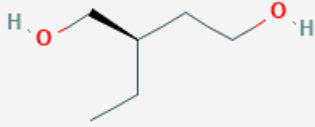
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>26.94</p> <p>Different pattern</p>		<p>C₅H₁₀O</p> <p>MWT = 86.055</p>	<p>Proposal #68</p> <p>BCJPEZMFAKOJPM-RFZPGFLSSA-N</p> <p>PUBCHEM Compound: 6427093</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>26.94</p> <p>Different pattern</p>		<p>C₅H₁₀O</p> <p>MWT = 86.055</p>	<p>Proposal #69</p> <p>BCJPEZMFAKOJPM-WHFBIAKZSA-N</p> <p>PUBCHEM Compound: 13357413</p>	<p>Availability of NMR-Data in CSEARCH</p> 

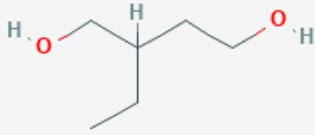


Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
26.99	 <p>The structure shows a three-membered cyclopropyl ring attached to an oxygen atom, which is further bonded to an ethyl group.</p>	$C_6H_{12}O$ MWT = 100.066	Proposal #70 FSYJSAIZYLQM-UHFFFAOYSA-N PUBCHEM Compound: 53642689	
27.34	 <p>The structure shows a cyclopropyl ring with two methyl groups on one carbon and a 1-hydroxyethyl group on another carbon.</p>	$C_7H_{14}O$ MWT = 114.077	Proposal #71 SIFLEUDKOSRPAP-UHFFFAOYSA-N PUBCHEM Compound: 14202705	



Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>27.38</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #72</p> <p>YYJCIRVETUQAIB-ZETCQYMHSA-N</p> <p>PUBCHEM Compound: 89694917</p>	
<p>27.38</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #73</p> <p>YYJCIRVETUQAIB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 10844367</p>	

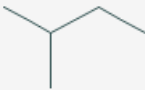

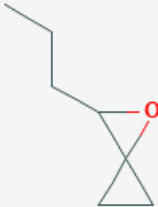
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>27.39</p> <p>Different pattern</p>		<p>C₇H₁₆O</p> <p>MWT = 116.077</p>	<p>Proposal #74</p> <p>YNPVNLWKVZZBTM-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 98346</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>27.39</p> <p>Different pattern</p>		<p>C₇H₁₆O</p> <p>MWT = 116.077</p>	<p>Proposal #75</p> <p>YNPVNLWKVZZBTM-ZETCQYMHSA-N</p> <p>PUBCHEM Compound: 13463446</p>	<p>Availability of NMR-Data in CSEARCH</p> 

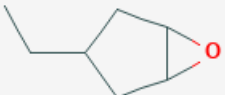
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>27.39</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #76</p> <p>YNPVNLWKVZZBTM-SSDOTTSWSA-N</p> <p>PUBCHEM Compound: 13463447</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>27.66</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #77</p> <p>CYVMBANVYOZFIG-LURJTMIESA-N</p> <p>PUBCHEM Compound: 12648202</p>	

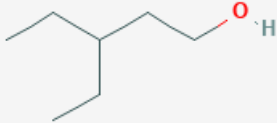

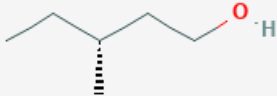

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p data-bbox="190 655 259 679">27.66</p> <p data-bbox="125 716 327 740">Different pattern</p>	 <p>The diagram shows the chemical structure of 2-ethylbutane-1,3-diol. It consists of a four-carbon main chain with hydroxyl groups on the first and third carbons, and an ethyl group on the second carbon. The hydroxyl groups are shown with dashed bonds to the carbons, indicating they are on the same side of the chain.</p>	<p data-bbox="1032 592 1137 616">$C_6H_{14}O_2$</p> <p data-bbox="992 655 1178 679">MWT = 118.066</p>	<p data-bbox="1458 549 1621 572">Proposal #78</p> <p data-bbox="1317 639 1753 663">CYMBANVYOZFIG-ZCFIWIBFSA-N</p> <p data-bbox="1335 700 1742 724">PUBCHEM Compound: 11804732</p>	

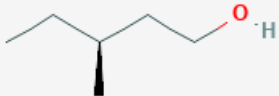

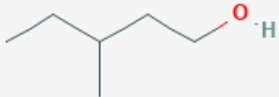

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>27.66</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #79</p> <p>CYVMBANVYOZFIG-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12648201</p>	
<p>27.72</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #80</p> <p>ZNAFWUJVHNGIE-NKWVEPMBSA-N</p> <p>PUBCHEM Compound: 13429647</p>	<p>Availability of NMR-Data in CSEARCH</p> 

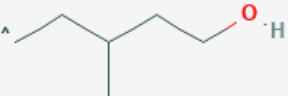
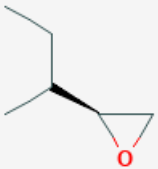

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
27.72 Different pattern		C ₇ H ₁₄ O MWT = 114.077	Proposal #81 ZNAFWUJVHNGIE-RQJHMYQMSA-N PUBCHEM Compound: 13429646	Availability of NMR-Data in CSEARCH 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
27.79	 	$C_7H_{18}O$ MWT = 118.077	Proposal #82 FOXQTCHXXJKLNK-UHFFFAOYSA-N PUBCHEM Compound: 21646453	
27.94 Different pattern		$C_7H_{12}O$ MWT = 112.077	Proposal #83 REZDAVHPQKKTGM-UHFFFAOYSA-N PUBCHEM Compound: 87130811	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
28.10 Different pattern	 The structure shows a cyclopropane ring with an oxygen atom bridged across one of the C-C bonds, forming an epoxide. An ethyl group is attached to the second carbon of the ring.	C ₇ H ₁₂ O MWT = 112.077	Proposal #84 PTTGXCWXVYMEBV-UHFFFAOYSA-N PUBCHEM Compound: 88554936	

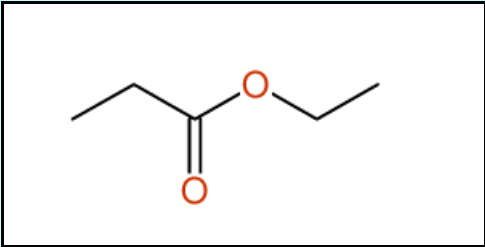
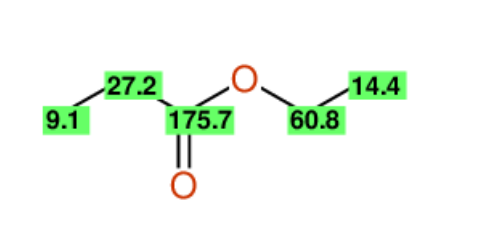
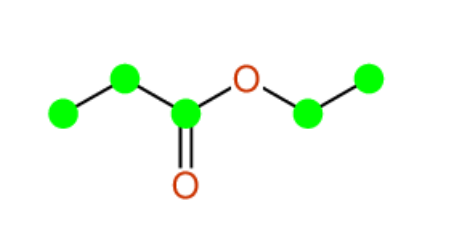
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>28.26</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #85</p> <p>DVEFUHVWVWJONKR-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 641005</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>28.44</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #86</p> <p>IWTBVKIGCDZRPL-ZCFIWIBFSA-N</p> <p>PUBCHEM Compound: 6999792</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>28.44</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #87</p> <p>IWTBVKIGCDZRPL-LURJTMIESA-N</p> <p>PUBCHEM Compound: 641003</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>28.44</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #88</p> <p>IWTBVKIGCDZRPL-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 11508</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>28.44</p> <p>Different pattern</p>		<p>$C_6H_{13}O$</p> <p>MWT = 101.066</p>	<p>Proposal #89</p> <p>FCACGIMTGMLTKJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57432776</p>	
<p>28.95</p> <p>Different pattern</p>		<p>$C_6H_{12}O$</p> <p>MWT = 100.066</p>	<p>Proposal #90</p> <p>OVFUAYYHQWUHCD-PRJDIBJQSA-N</p> <p>PUBCHEM Compound: 86758958</p>	<p>Availability of NMR-Data in CSEARCH</p> 

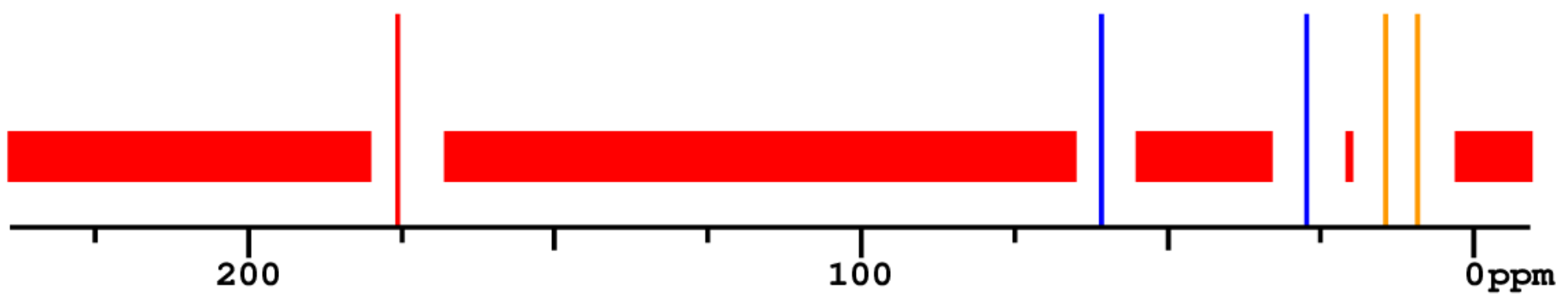
Detailed Analysis

Structure Proposal #1

Structure	Similarity Measure
 <p>Chemical structure of ethyl propyl ketone (CH₃CH₂COCH₂CH₃).</p>	<p>Deviation = 0.87 ppm</p> <p>C₅H₁₀O₂</p> <p>MWT = 102.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>FKRCODPIKNYEAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map
 <p>Chemical structure of ethyl propyl ketone with predicted chemical shift values (ppm):</p> <ul style="list-style-type: none">9.1 (methyl carbons)27.2 (methylene carbons)175.7 (carbonyl carbon)60.8 (methylene carbon adjacent to oxygen)14.4 (methyl carbon adjacent to oxygen)	 <p>Matching map showing the correspondence between the predicted chemical shift values and the atoms in the chemical structure.</p>

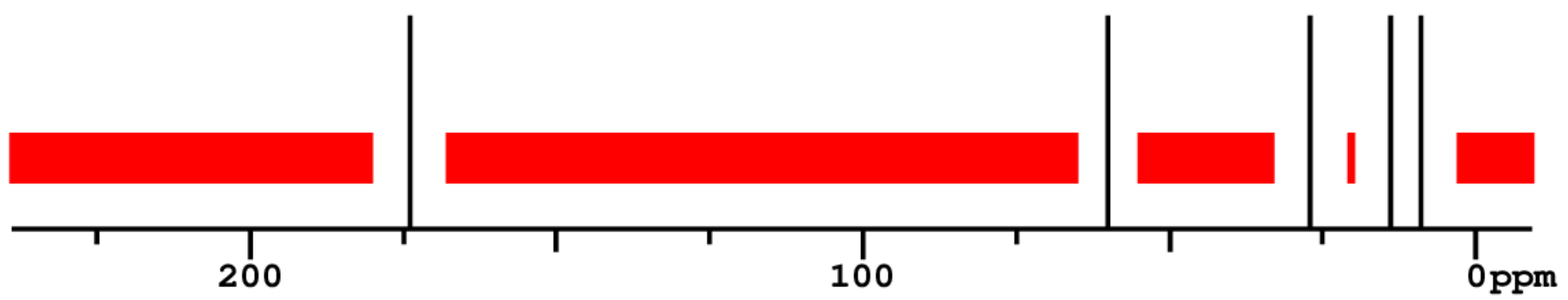
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

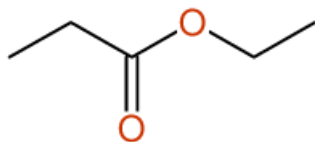
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[Back to Complete Result](#)

Structure Proposal #2

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_{10}O_2$

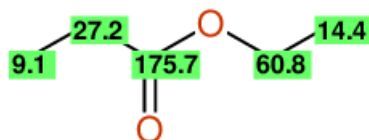
MWT = 100.06

[PUBCHEM](#)

Search Web for this structure:

[BYLOWUCDFUYIQ](#)

Predicted Chemical Shiftvalues

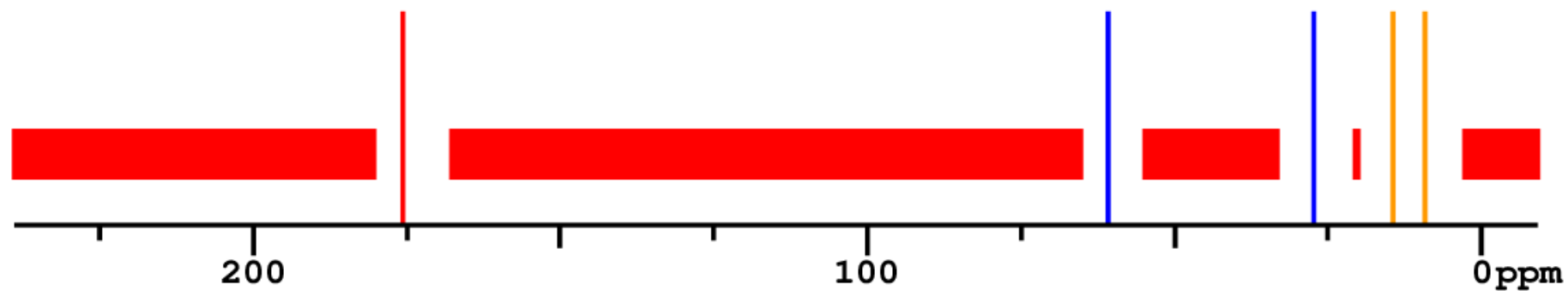


Matching Map



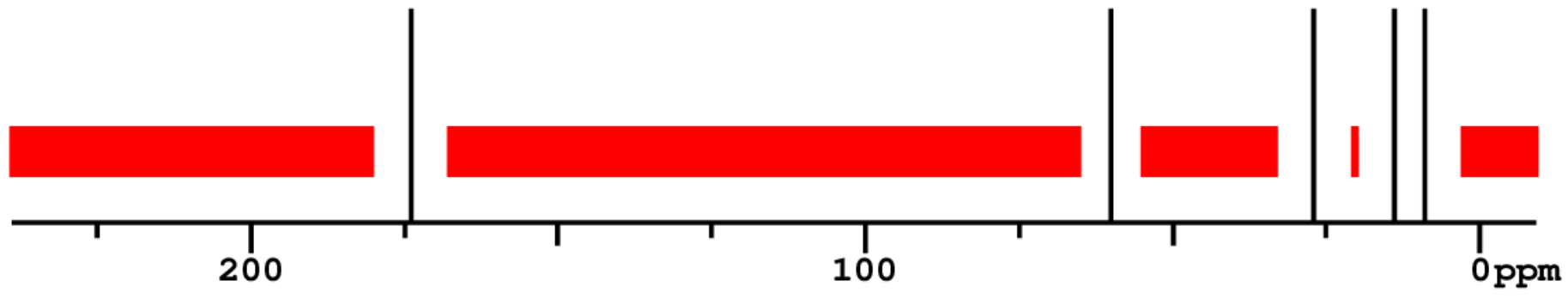
Predicted shift values

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



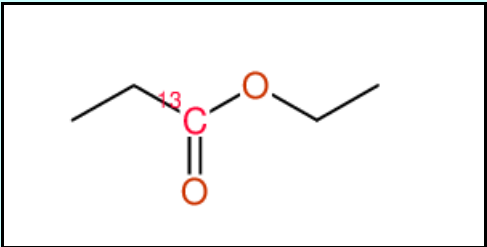
Experimental shift values

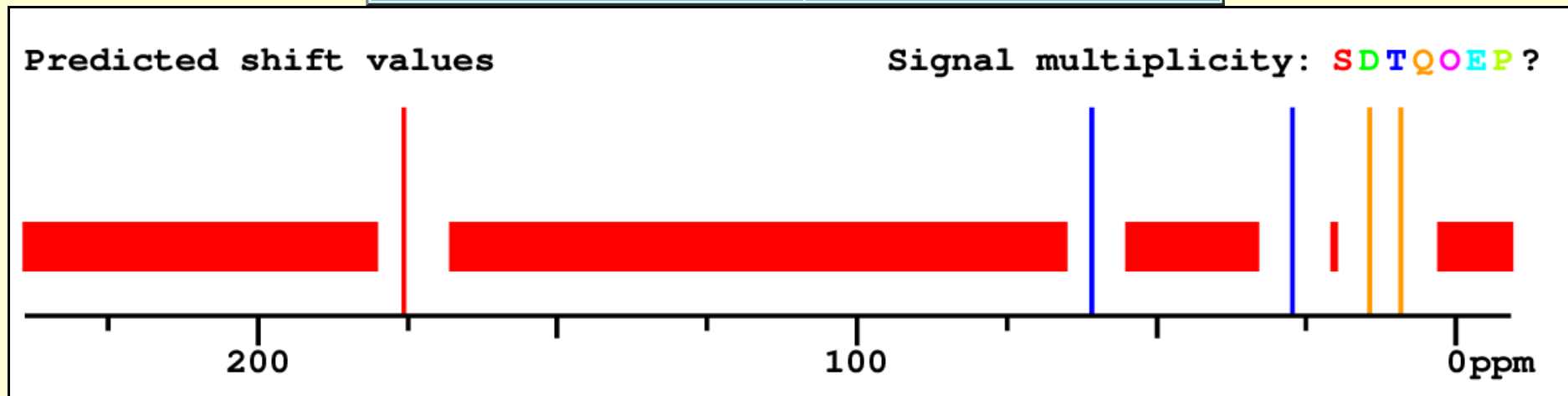
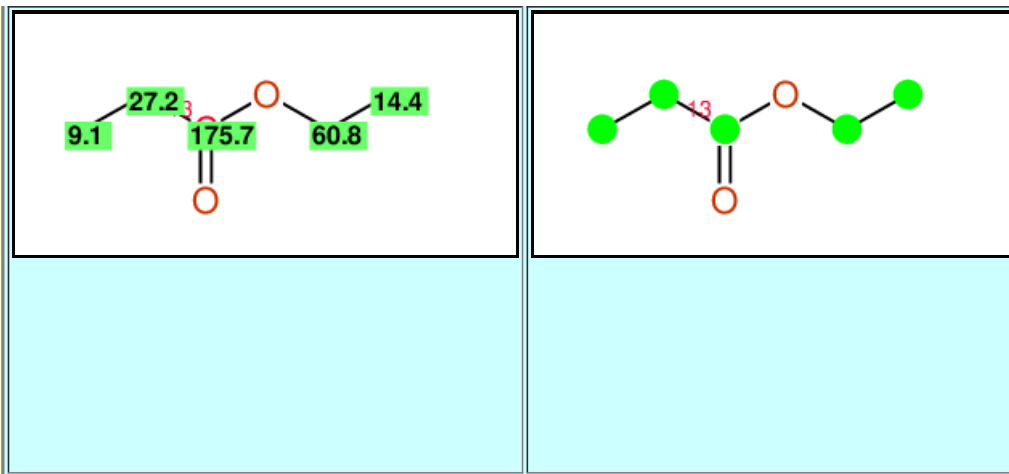
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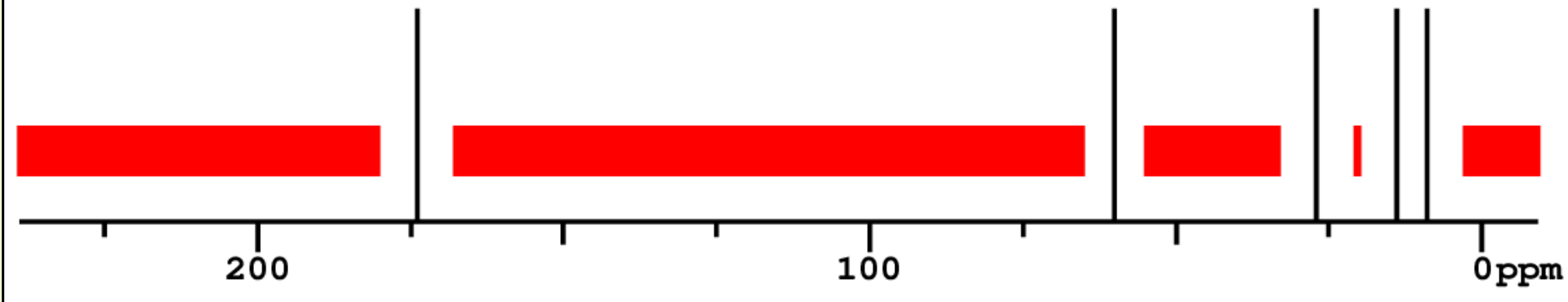
Structure Proposal #3

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 103.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>FKRCODPIKNYEAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



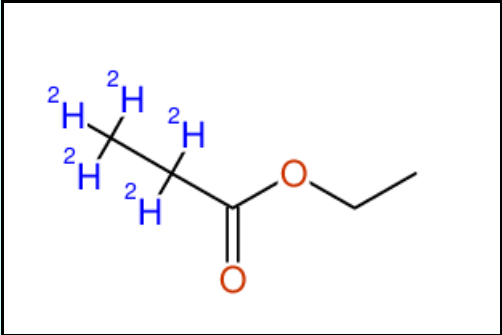
Experimental shift values

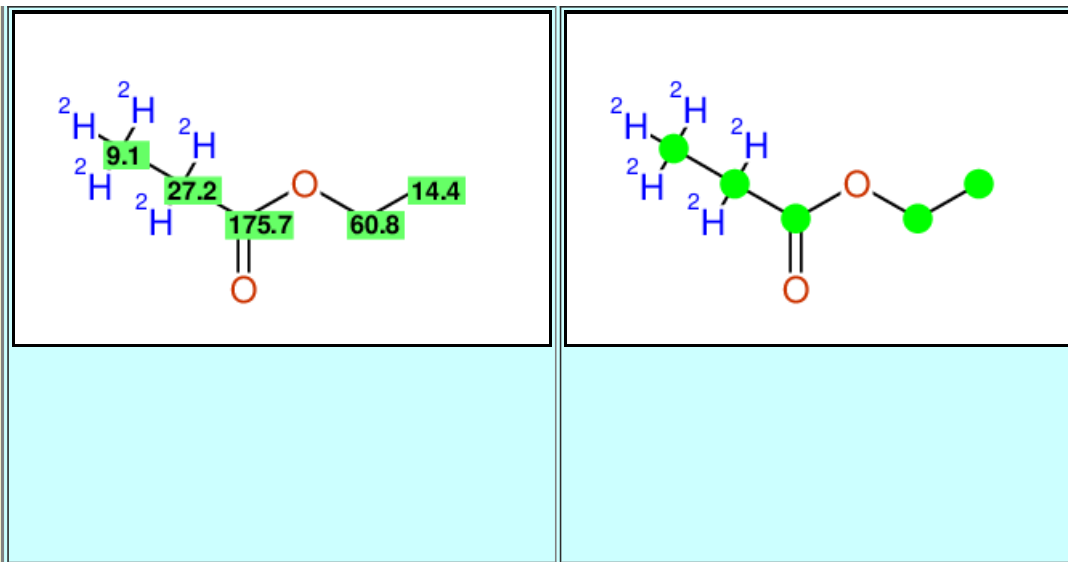
No line in reference: 



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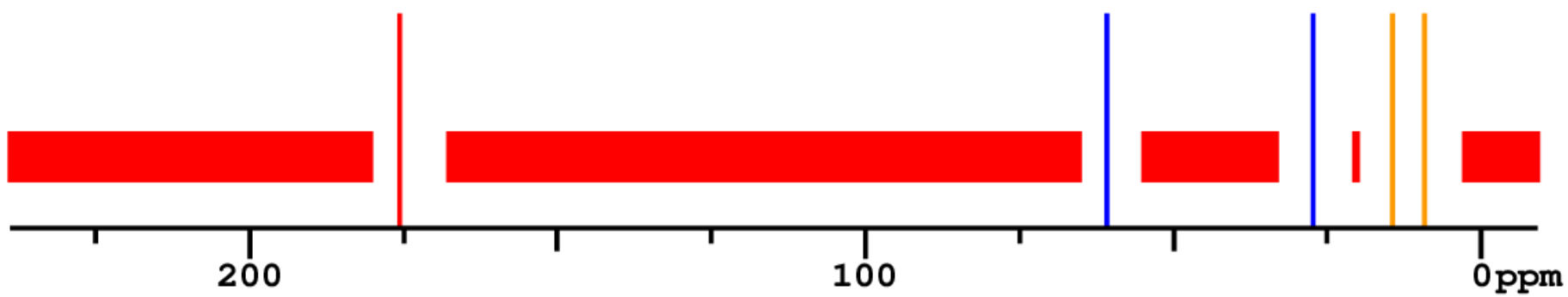
Structure Proposal #4

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 107.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>FKRCODPIKNYEAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map




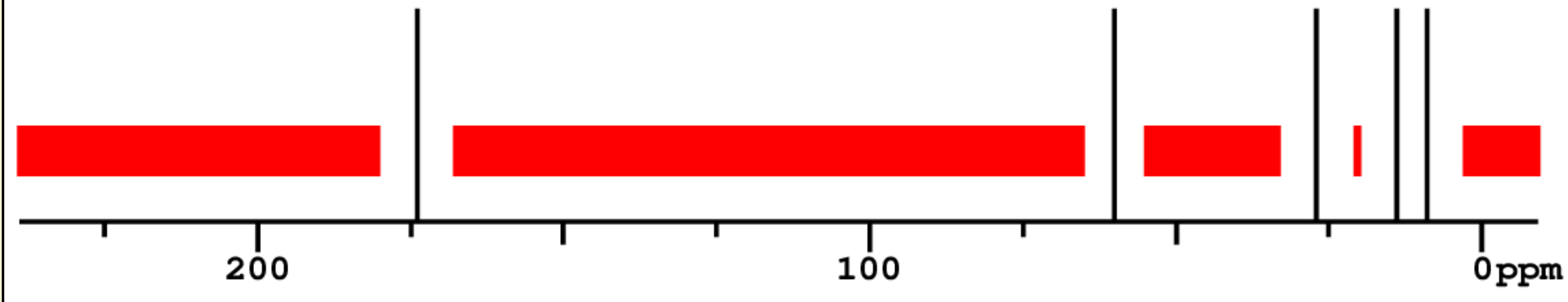
Predicted shift values

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



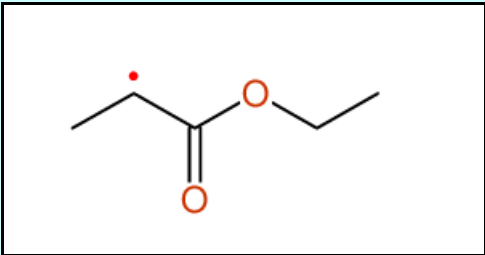
Experimental shift values

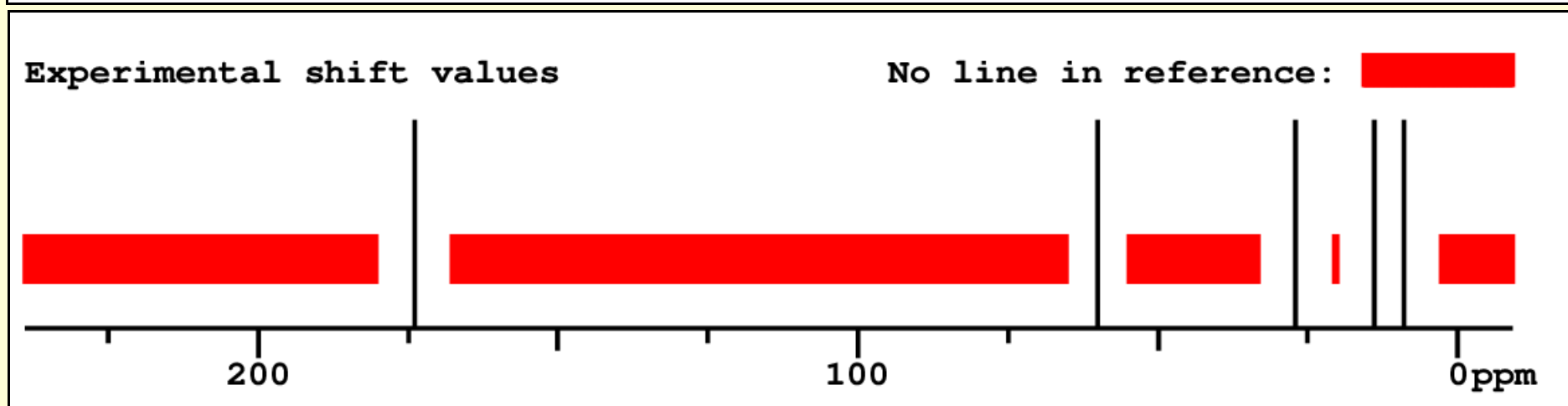
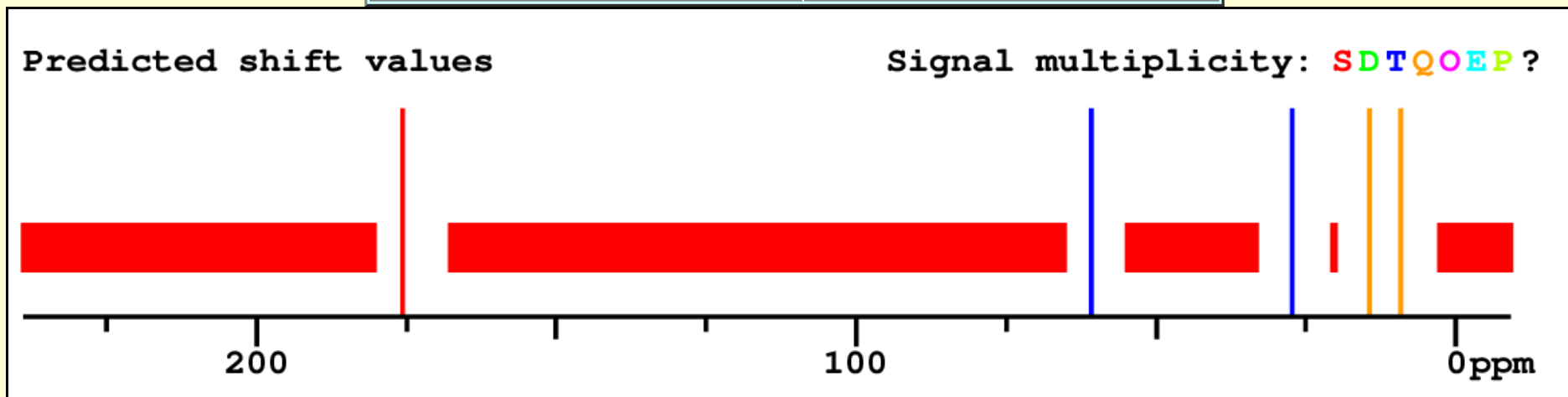
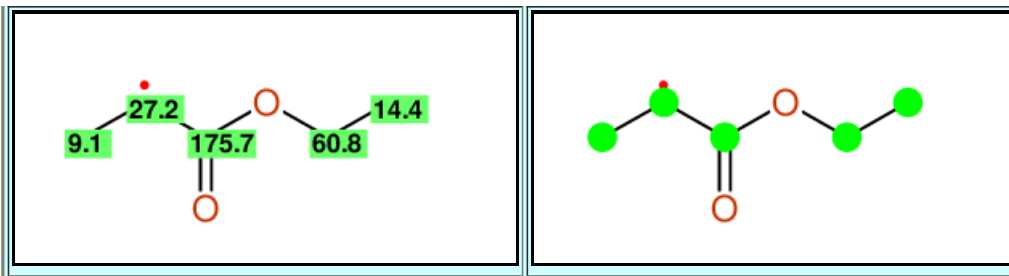
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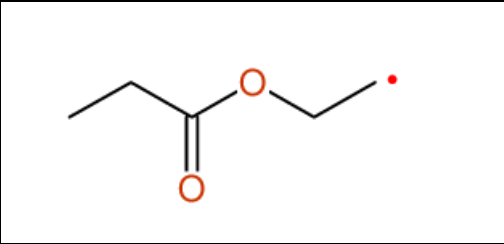
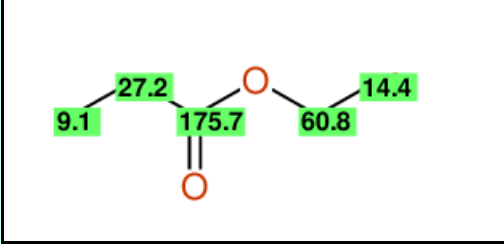
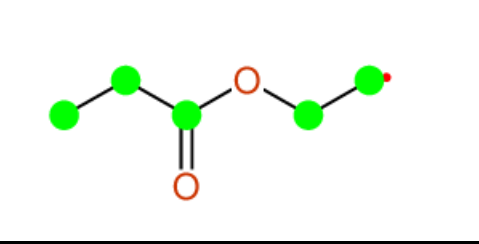
Structure Proposal #5

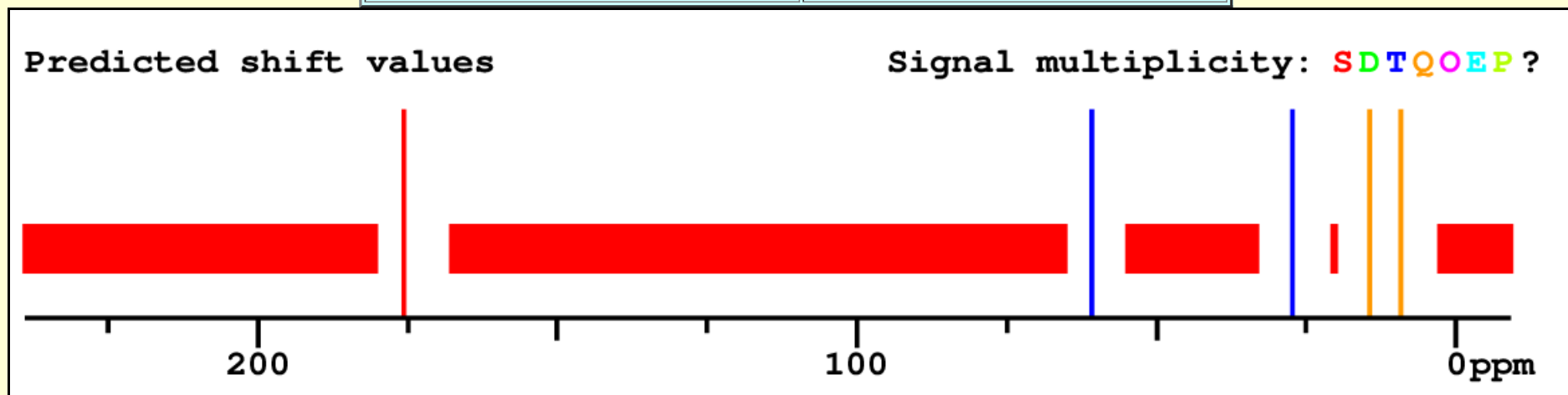
Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 101.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>UPRLWNPAOPKPCE</p>
Predicted Chemical Shiftvalues	Matching Map



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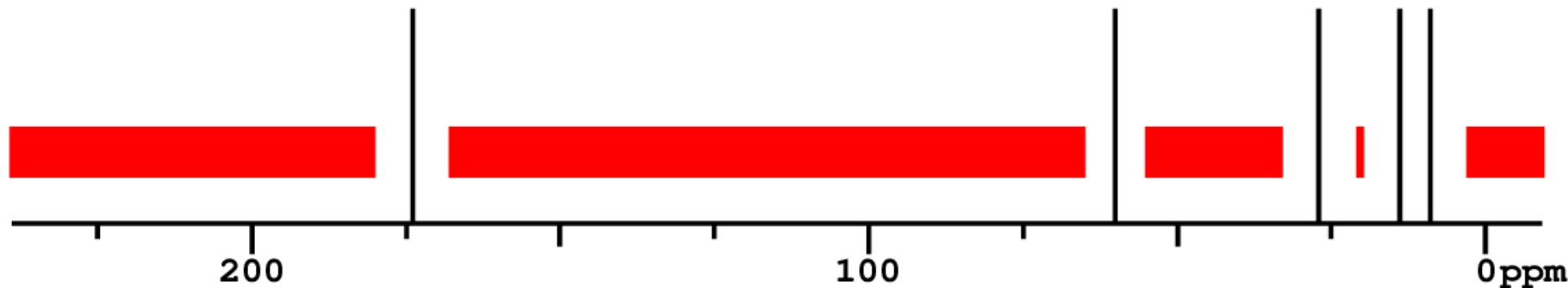
Structure Proposal #6

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_{10}O_2$ MWT = 101.06 PUBCHEM Search Web for this structure: IRGLFRDZYNBBCO
Predicted Chemical Shiftvalues	Matching Map
	



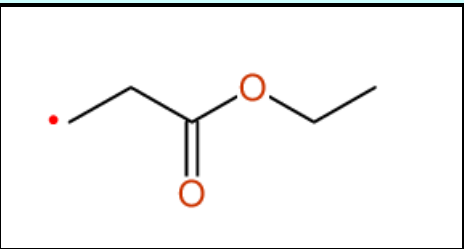
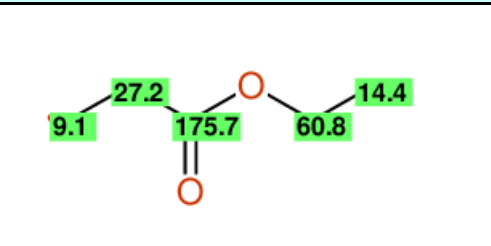
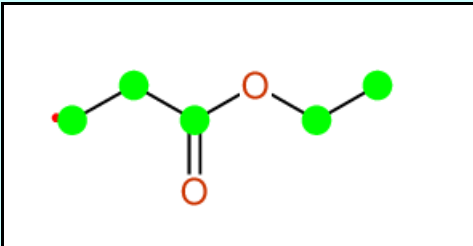
Experimental shift values

No line in reference: 



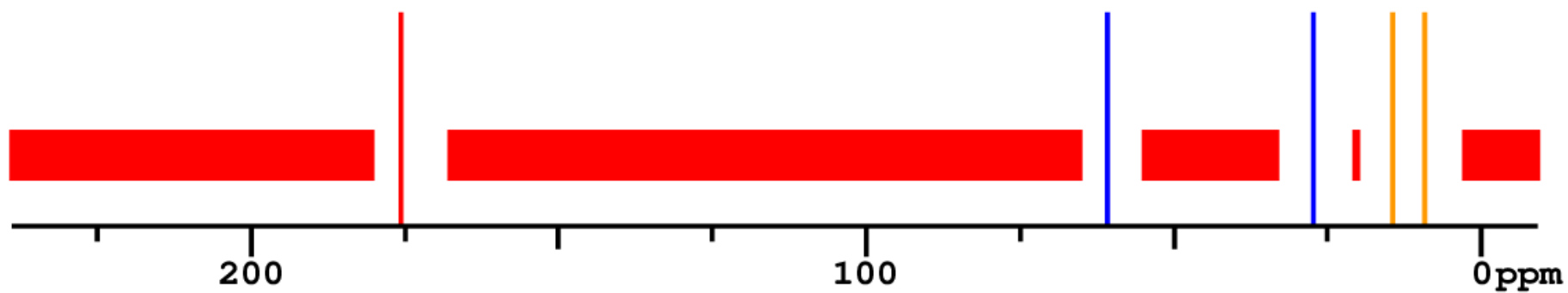
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Structure Proposal #7

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_{10}O_2$ MWT = 101.06 PUBCHEM Search Web for this structure: SOKCNILPAQLIRC
Predicted Chemical Shiftvalues	Matching Map
	

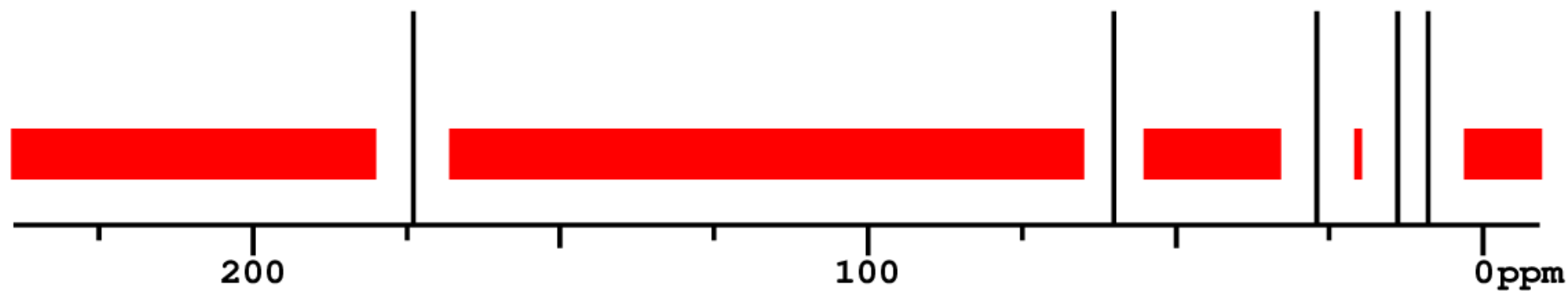
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

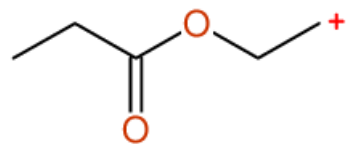
No line in reference: [red bar]



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Structure Proposal #8

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_9O_2^+$

MWT = 101.06

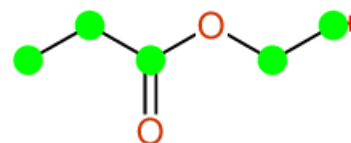
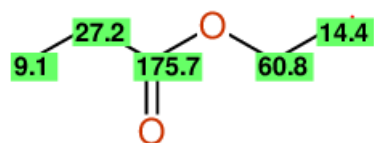
[PUBCHEM](#)

Search Web for this structure:

[GOKITYWXYBHPKU](#)

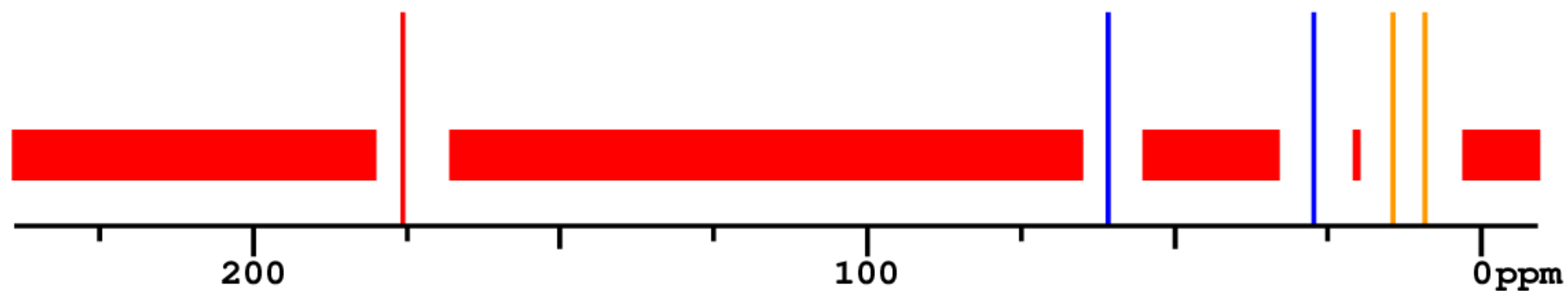
Predicted Chemical Shiftvalues

Matching Map



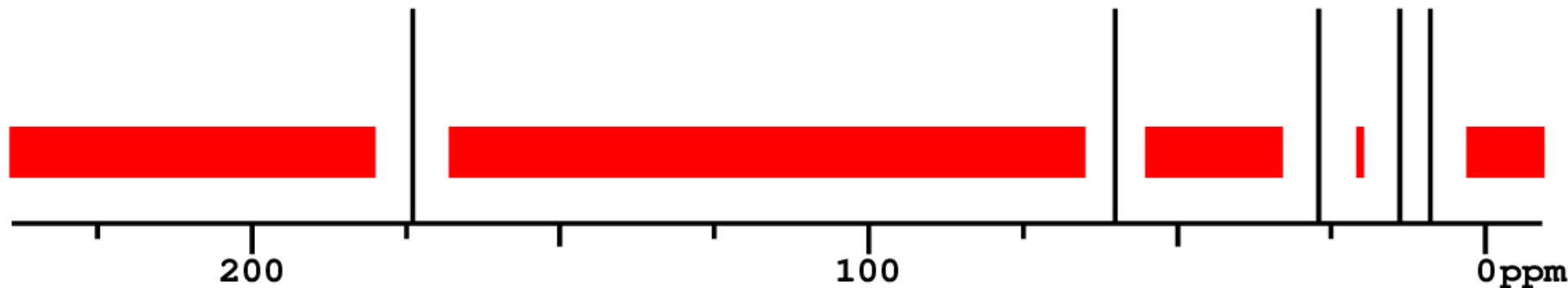
Predicted shift values

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



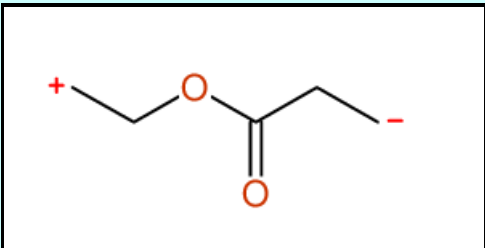
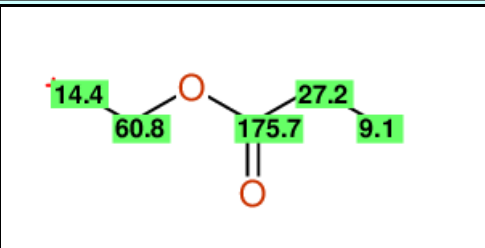
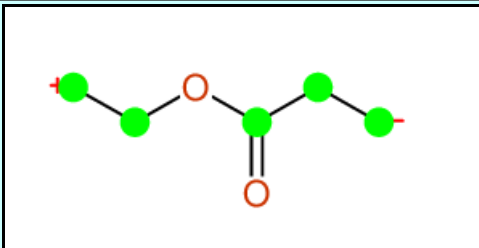
Experimental shift values

No line in reference: 



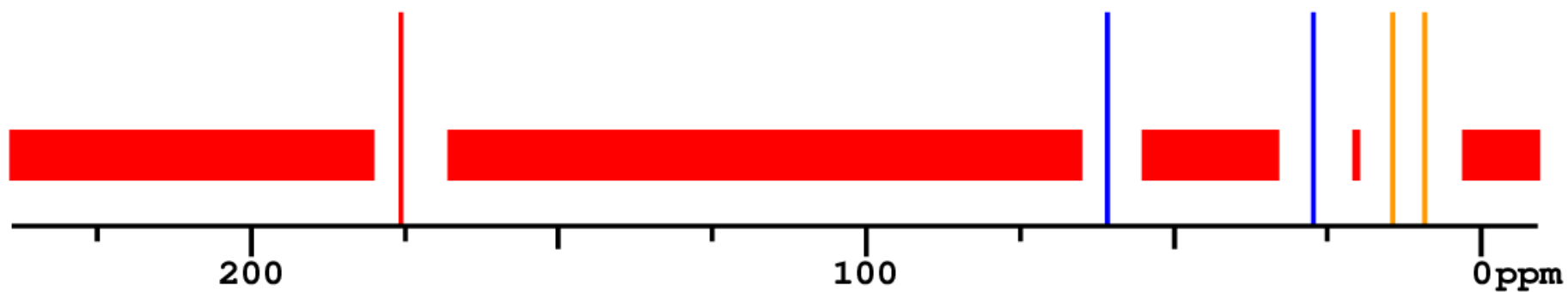
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Structure Proposal #9

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_8O_2$</p> <p>MWT = 100.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>LVCAAHDUTLIBML</p>
Predicted Chemical Shiftvalues	Matching Map
	

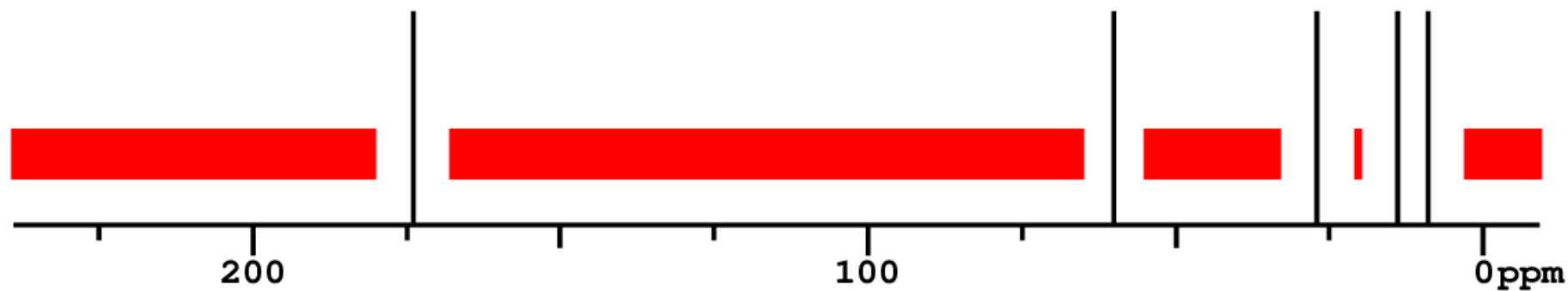
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

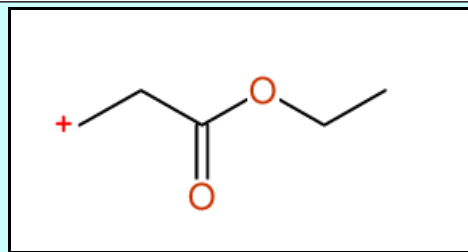
No line in reference: [red bar]



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Structure Proposal #10

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_9O_2^+$

MWT = 101.06

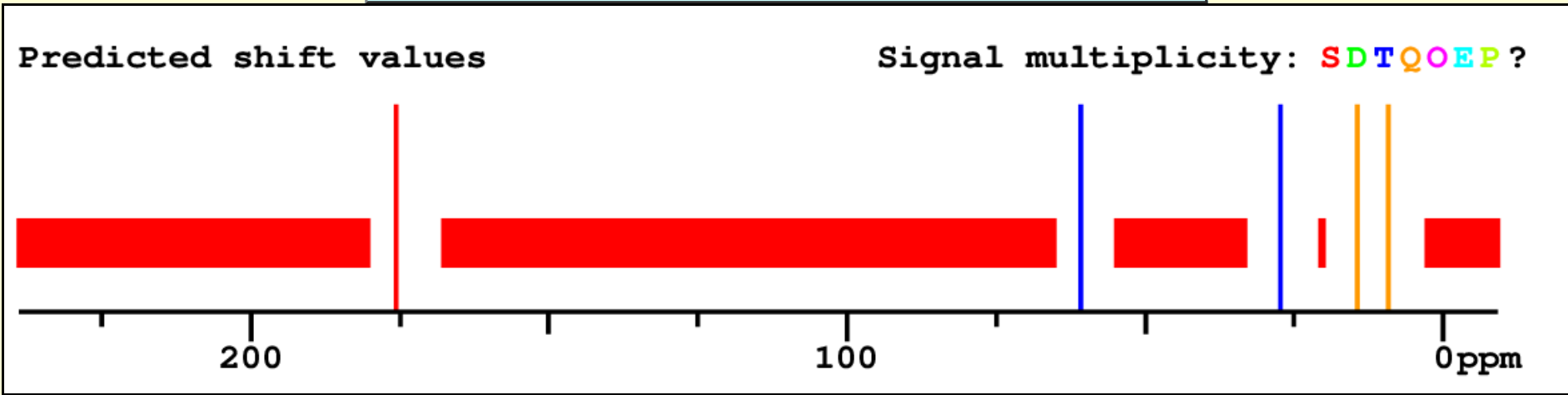
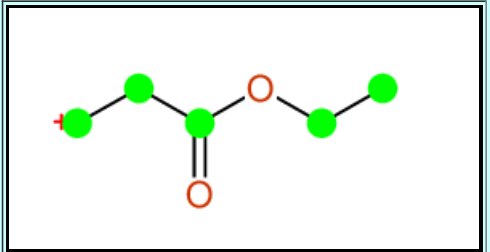
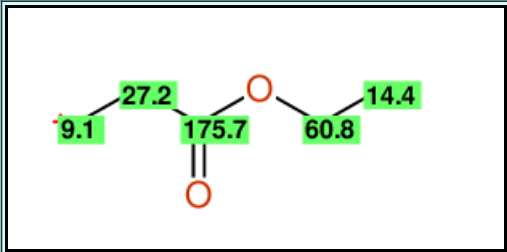
[PUBCHEM](#)

Search Web for this structure:


[MUQMZQYQIIZBIT](#)

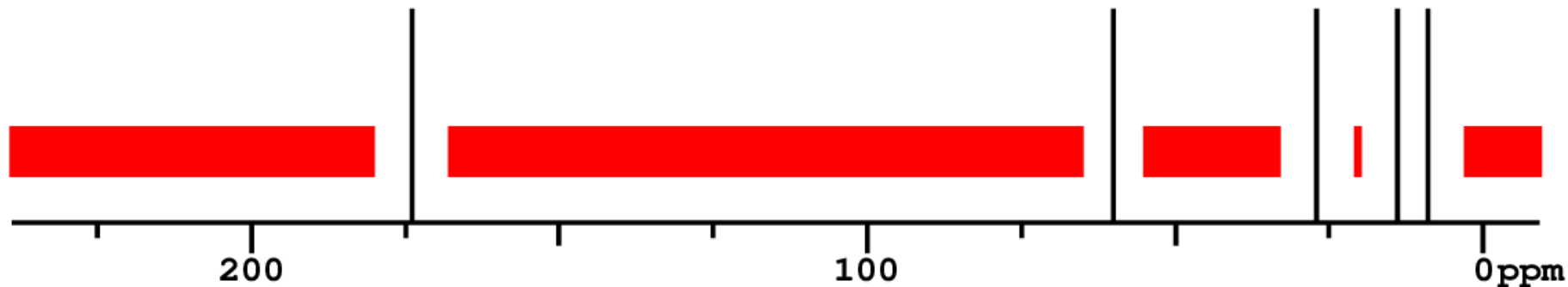
Predicted Chemical Shiftvalues

Matching Map



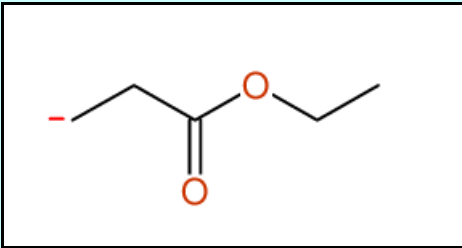
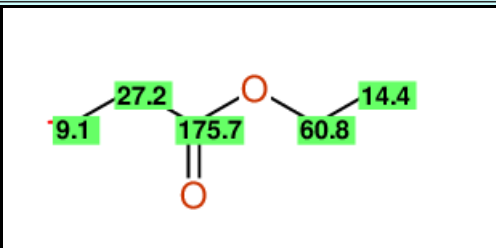
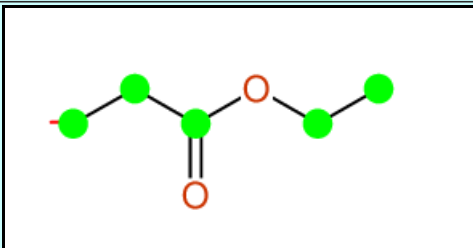
Experimental shift values

No line in reference: 



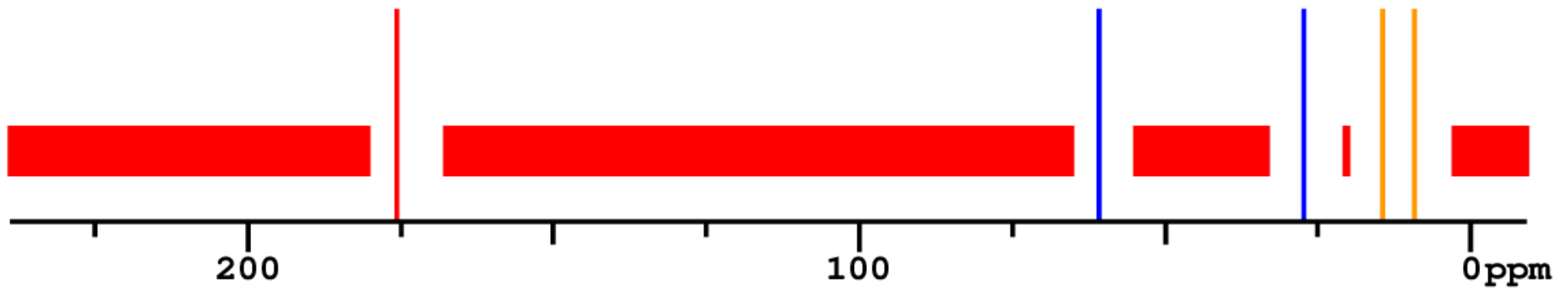
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Structure Proposal #11

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_9O_2^-$</p> <p>MWT = 101.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>NWIUUTFORIXPJC</p>
Predicted Chemical Shiftvalues	Matching Map
	

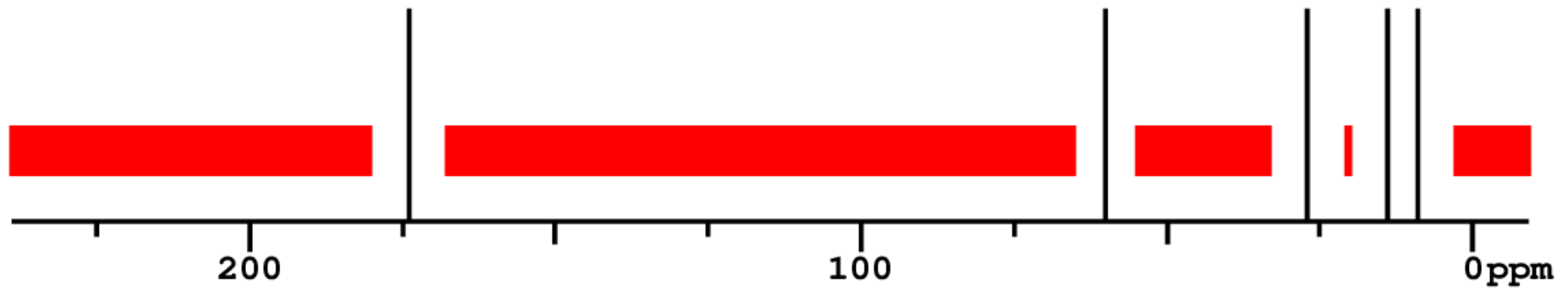
Predicted shift values

Signal multiplicity: S D T Q O E P ?



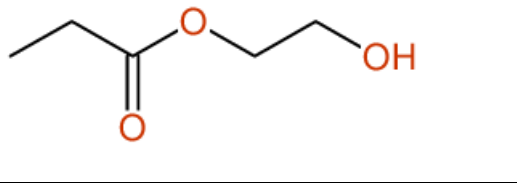
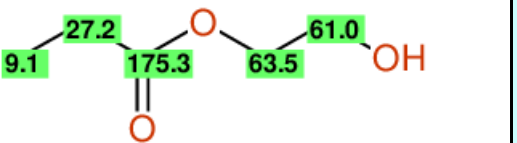
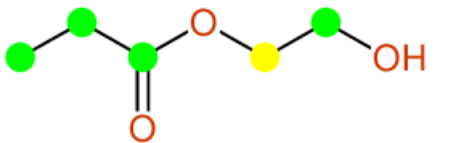
Experimental shift values

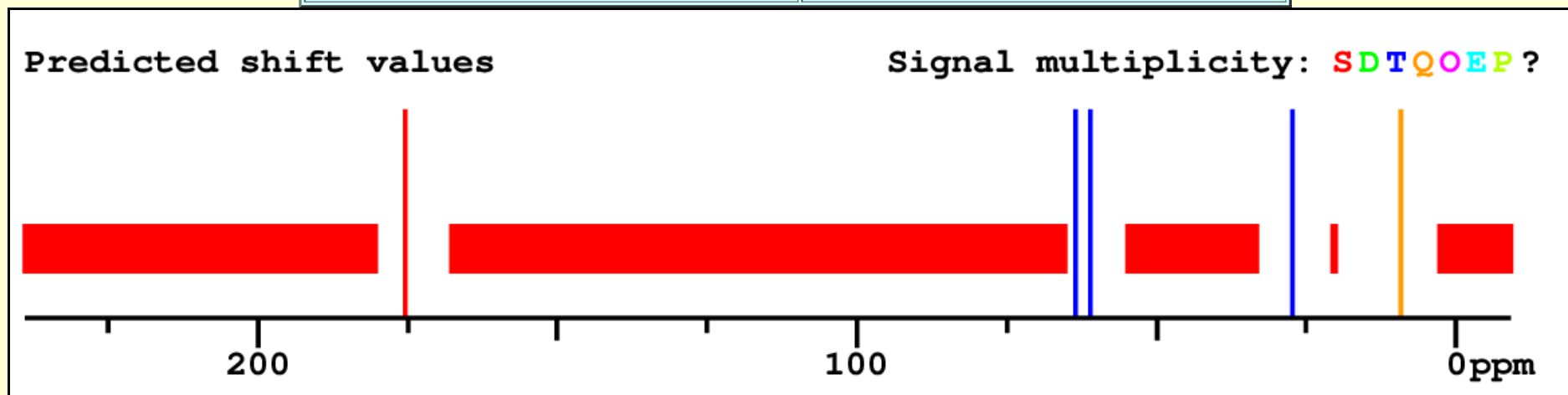
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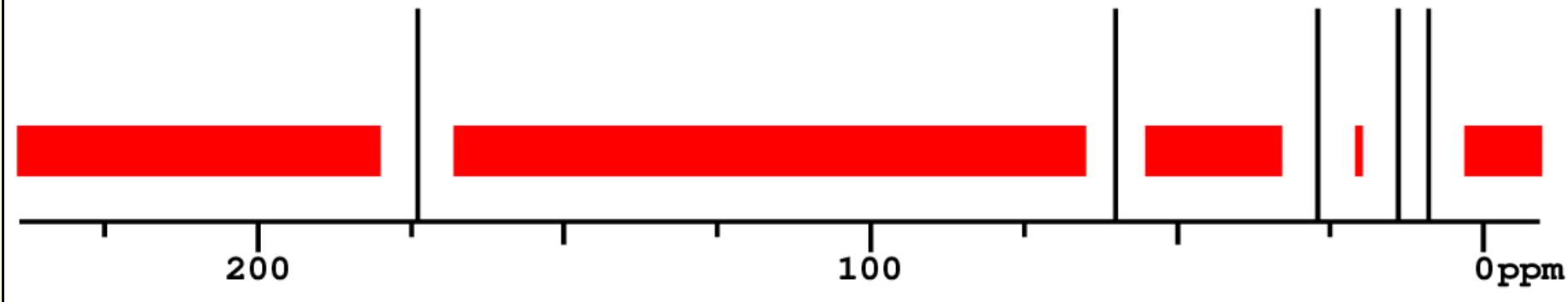
Structure Proposal #12

Structure	Similarity Measure
	Deviation = 2.02 ppm $C_5H_{10}O_3$ MWT = 118.06 PUBCHEM Search Web for this structure: SFAMKDPMPDEXGH
Predicted Chemical Shiftvalues	Matching Map
	



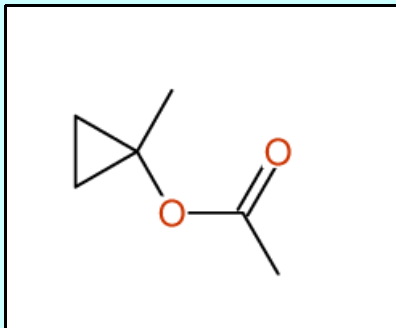
Experimental shift values

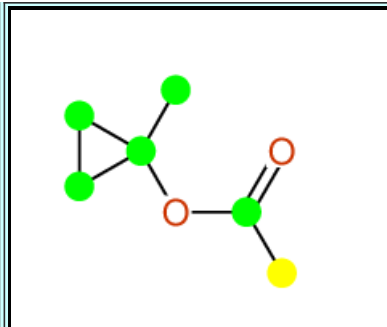
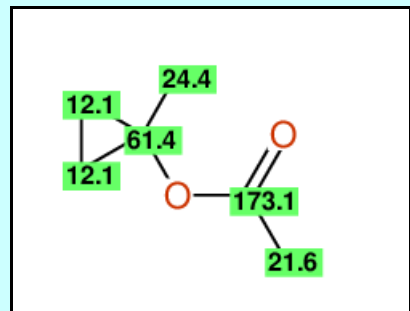
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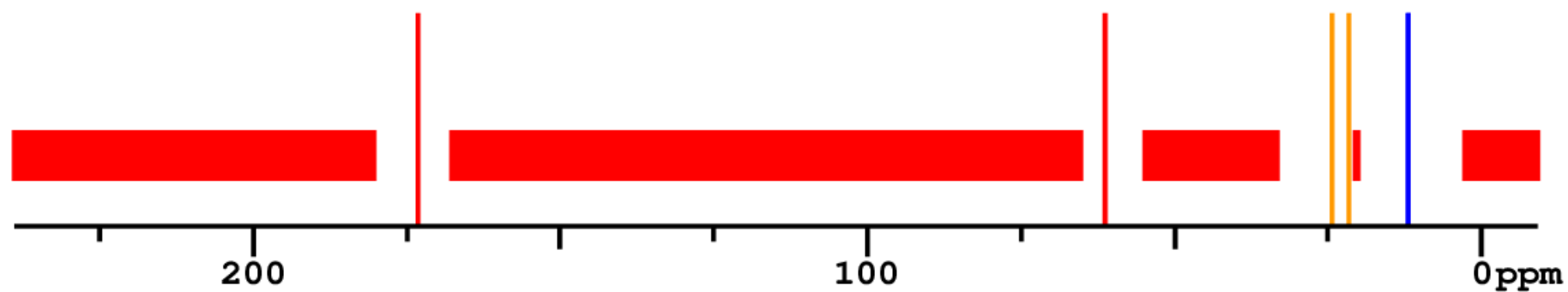
Structure Proposal #13

Structure	Similarity Measure
	<p>Deviation = 2.45 ppm</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>MJRMRENBUDEGM</p>
Predicted Chemical Shiftvalues	Matching Map



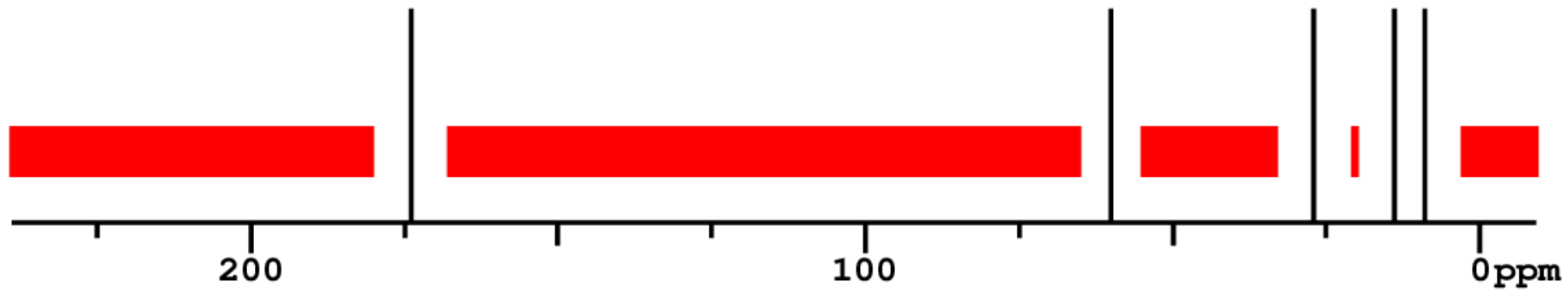
Predicted shift values

Signal multiplicity: S D T Q O E P ?



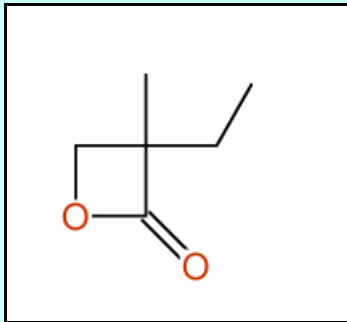
Experimental shift values

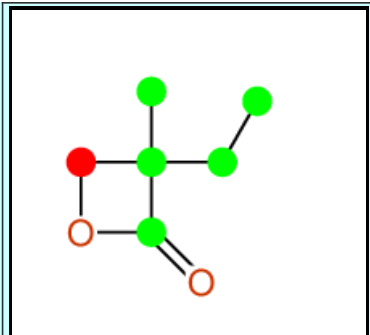
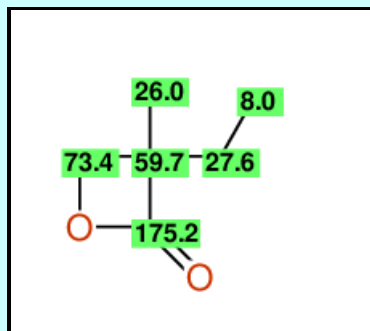
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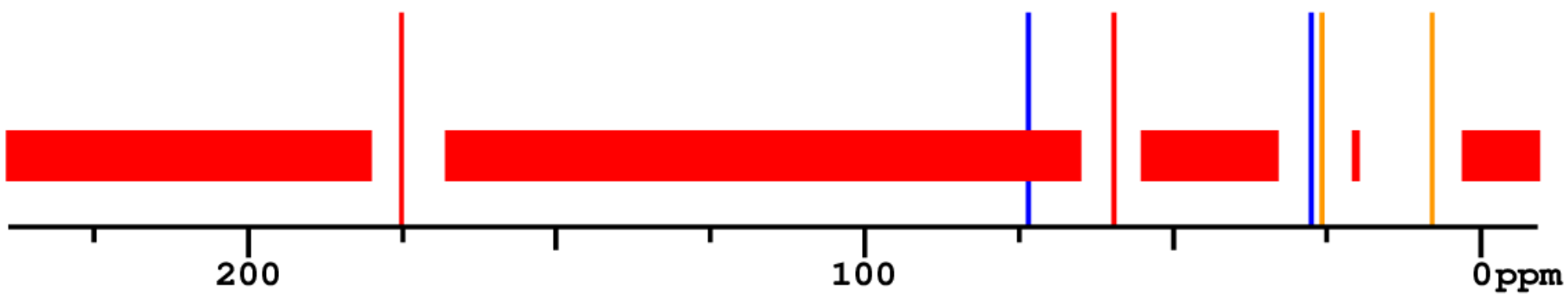
Structure Proposal #14

Structure	Similarity Measure
	<p>Deviation = 4.17 ppm (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>UFTRVHTYHBMWOF</p>
Predicted Chemical Shiftvalues	Matching Map



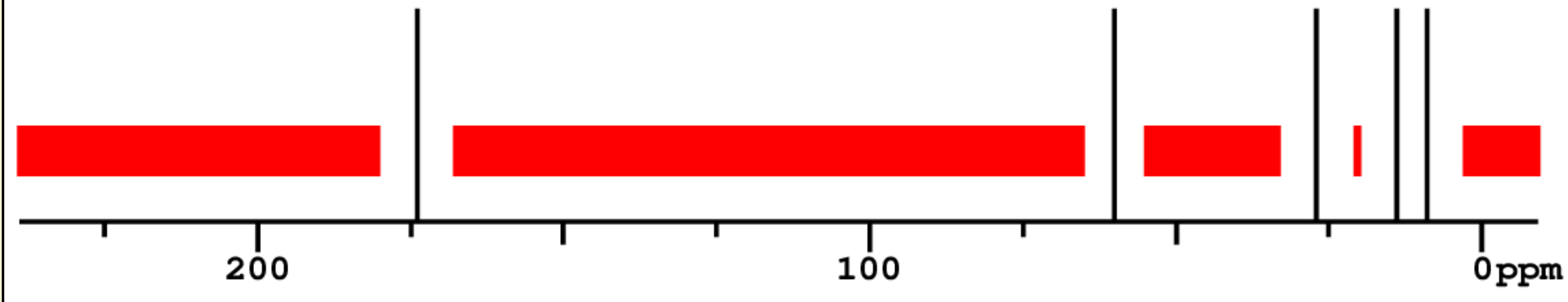
Predicted shift values

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



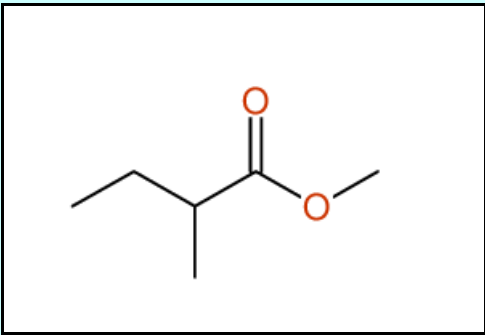
Experimental shift values

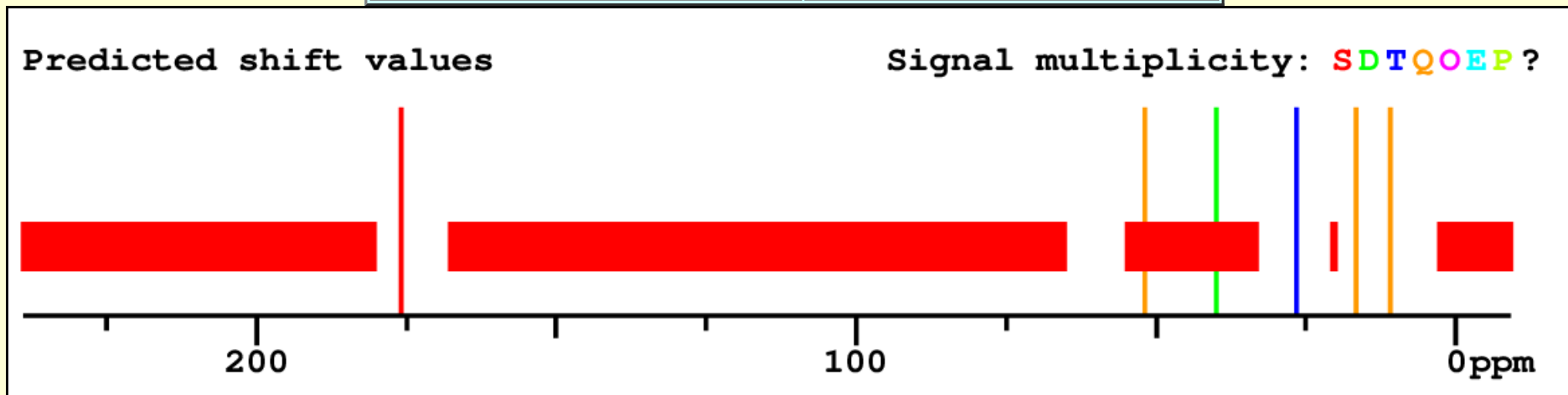
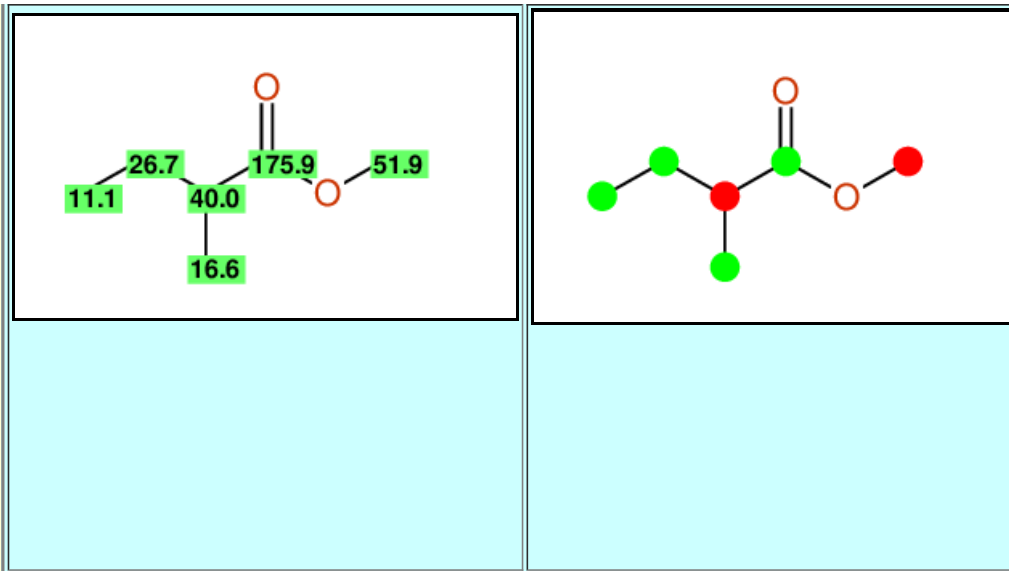
No line in reference: 




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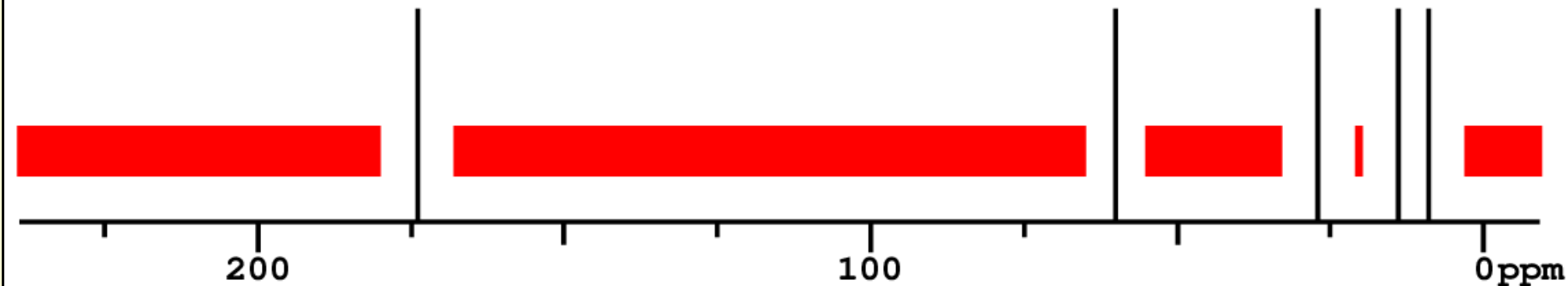
Structure Proposal #15

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>YMRCZGBILKTSC</p>
Predicted Chemical Shiftvalues	Matching Map



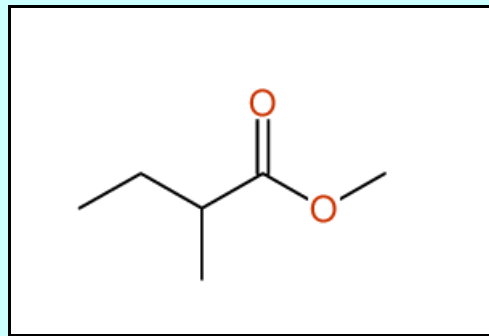
Experimental shift values

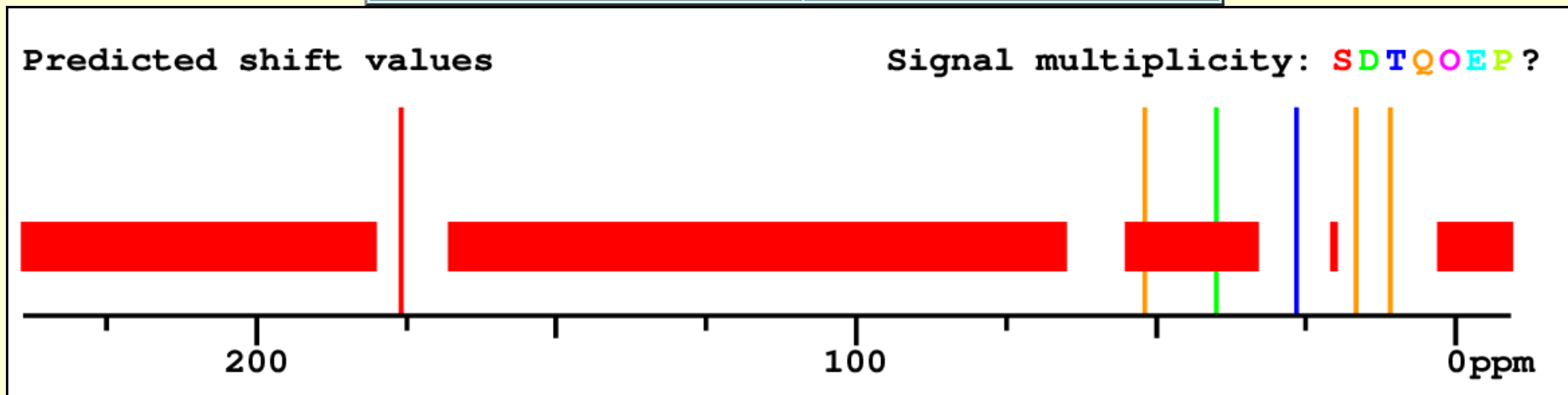
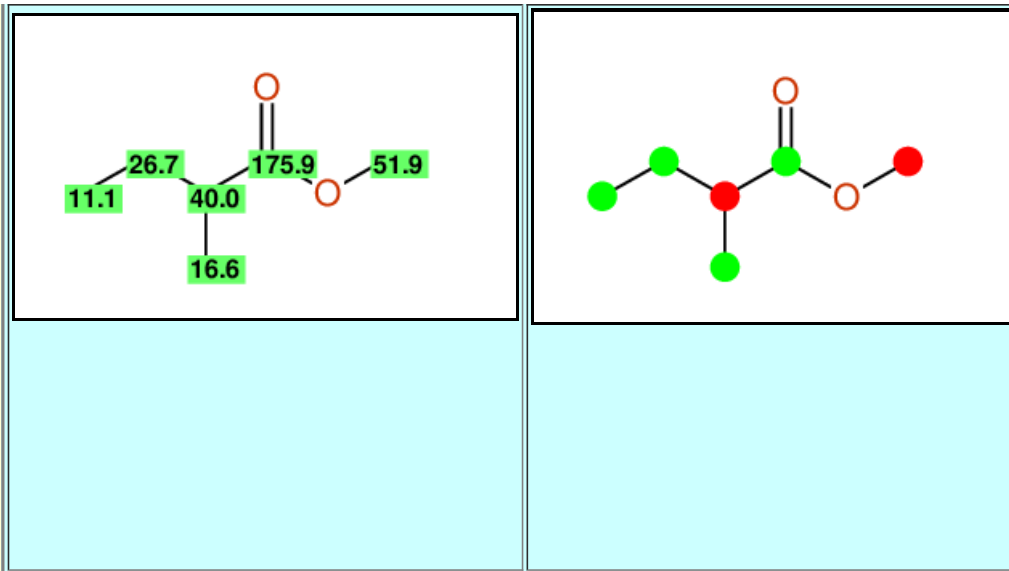
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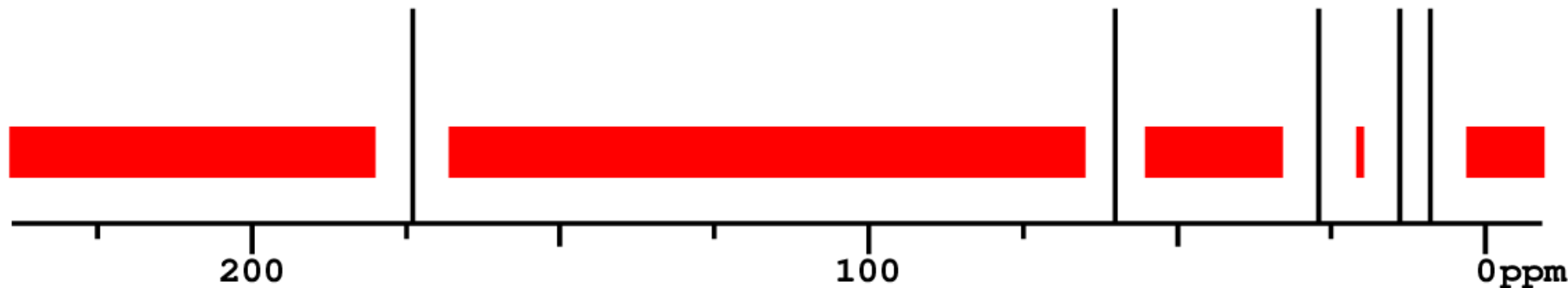
Structure Proposal #16

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure: OYGDMLWOJBKWLN</p>
Predicted Chemical Shiftvalues	Matching Map



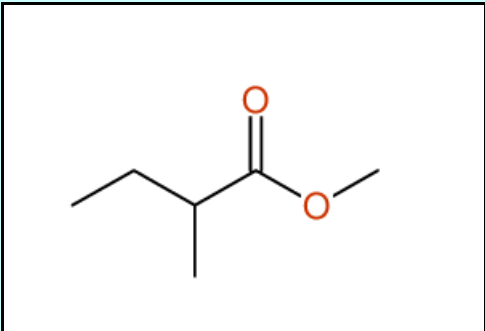
Experimental shift values

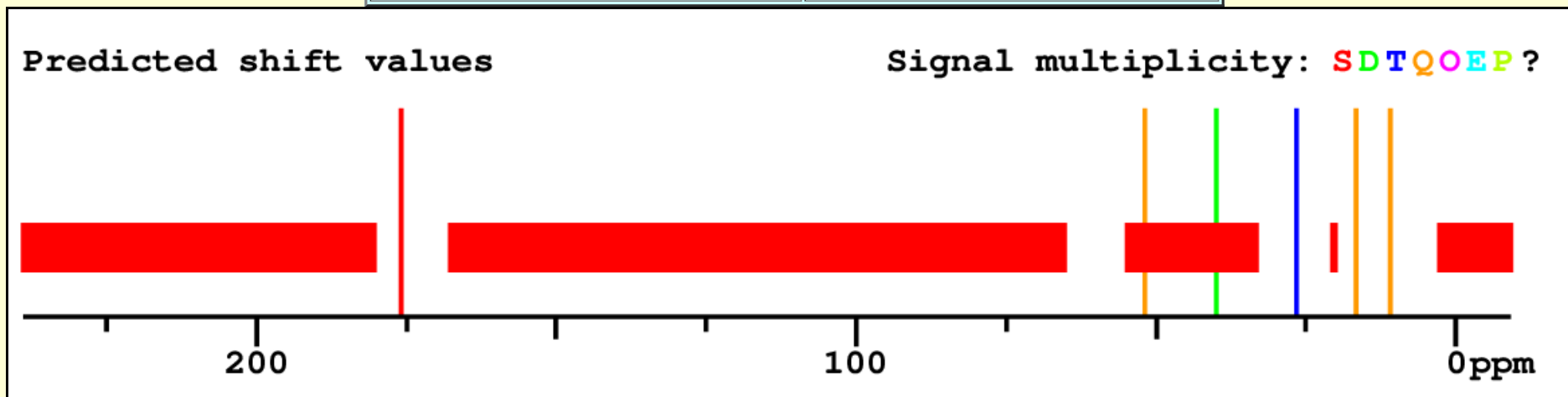
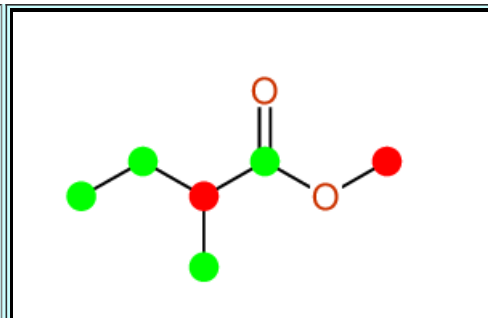
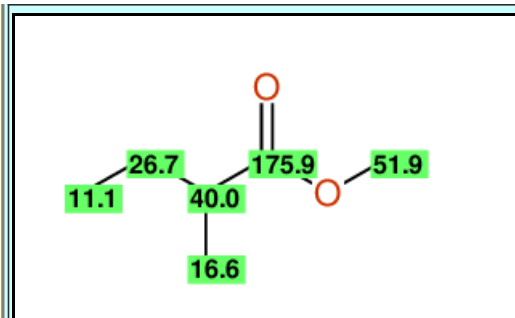
No line in reference: 



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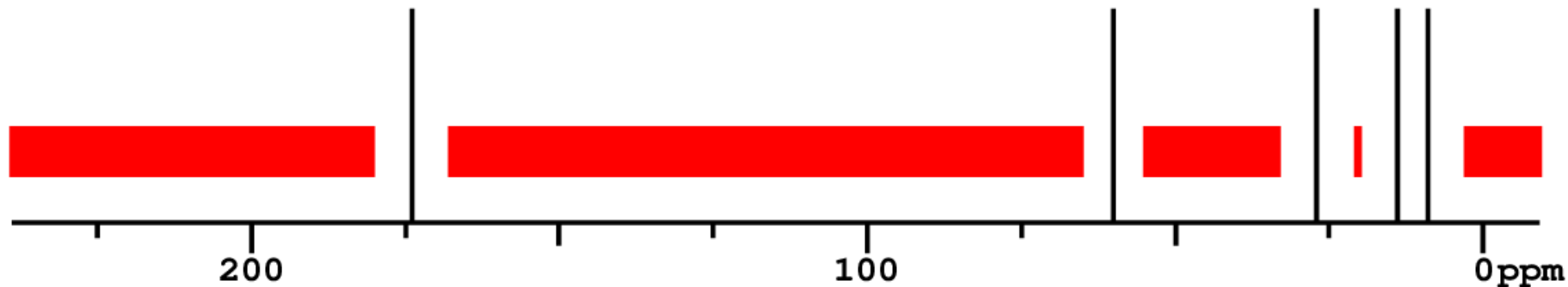
Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 116.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>OCWLYWIFNDCWRZ</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



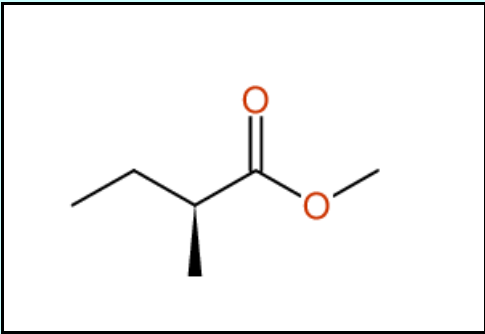
Experimental shift values

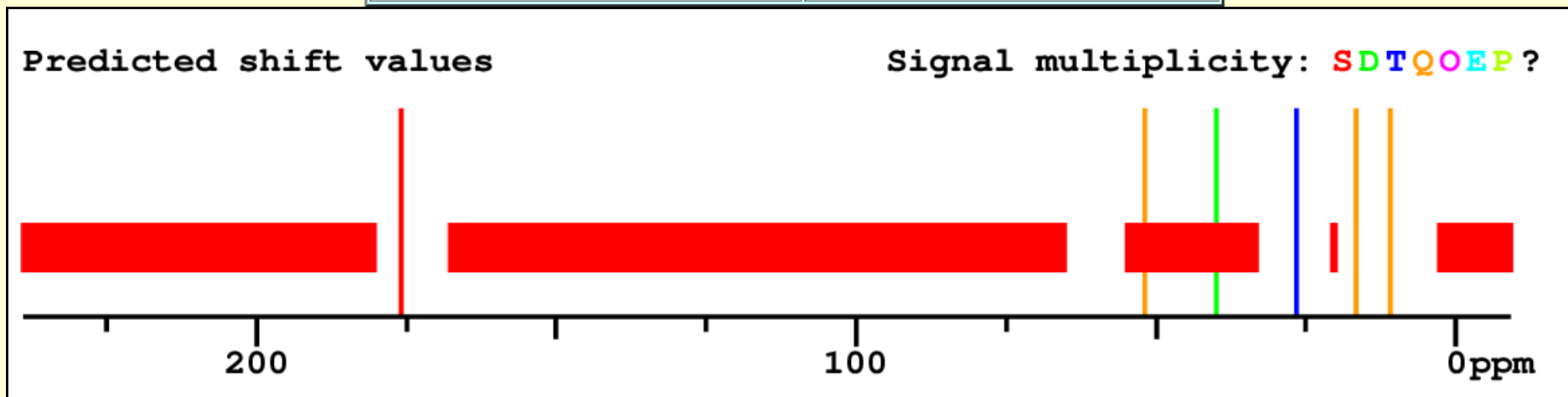
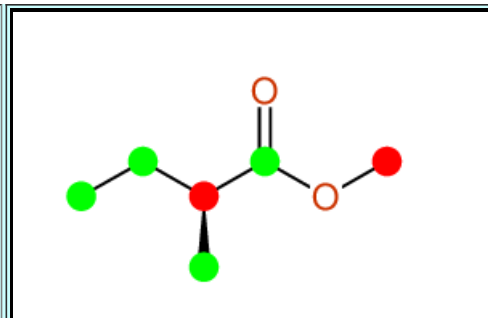
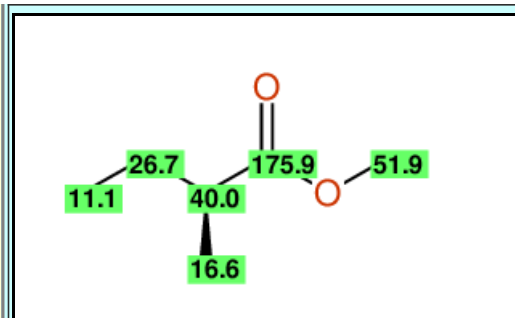
No line in reference: 




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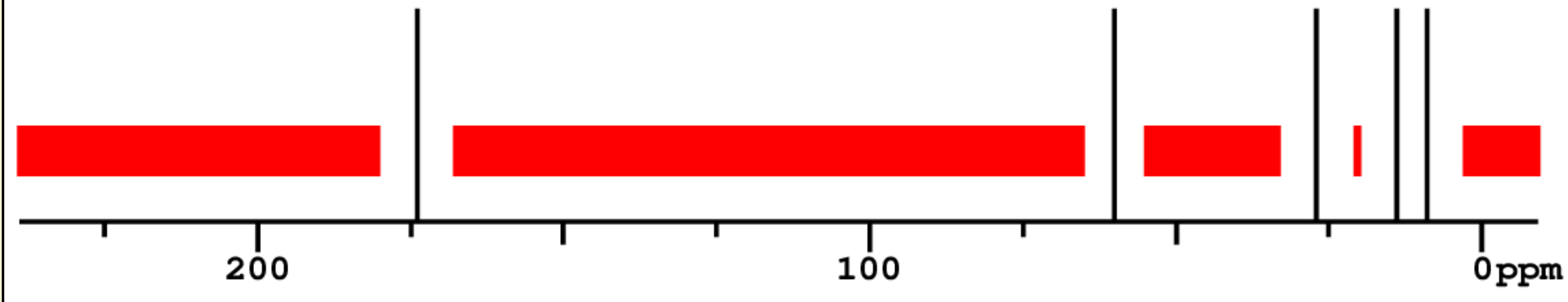
Structure Proposal #18

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 116.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>OCWLYWIFNDCWRZ</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



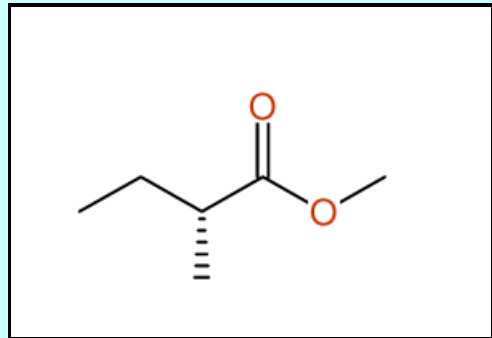
Experimental shift values

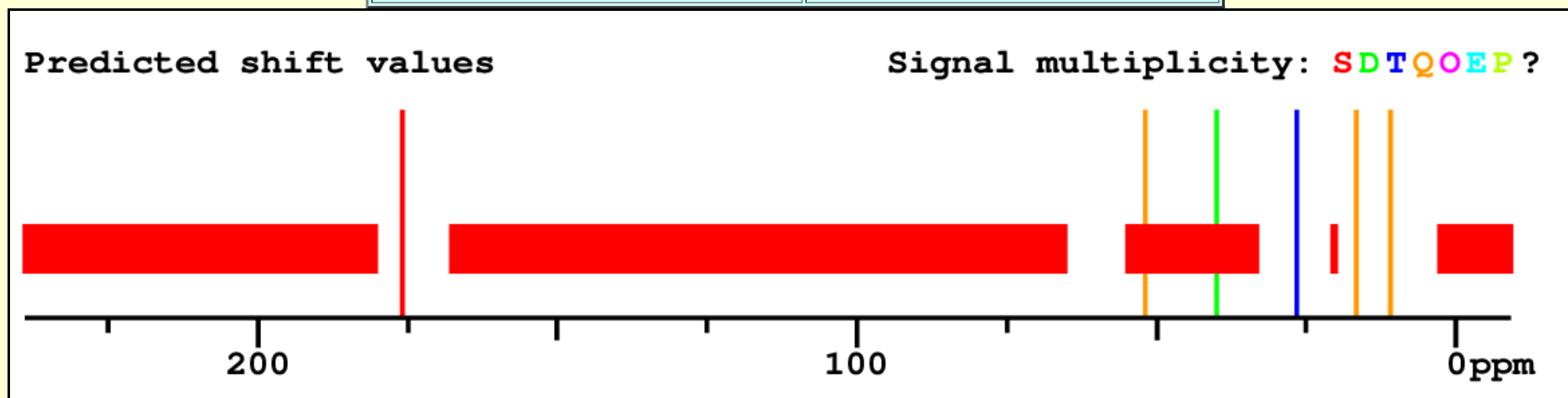
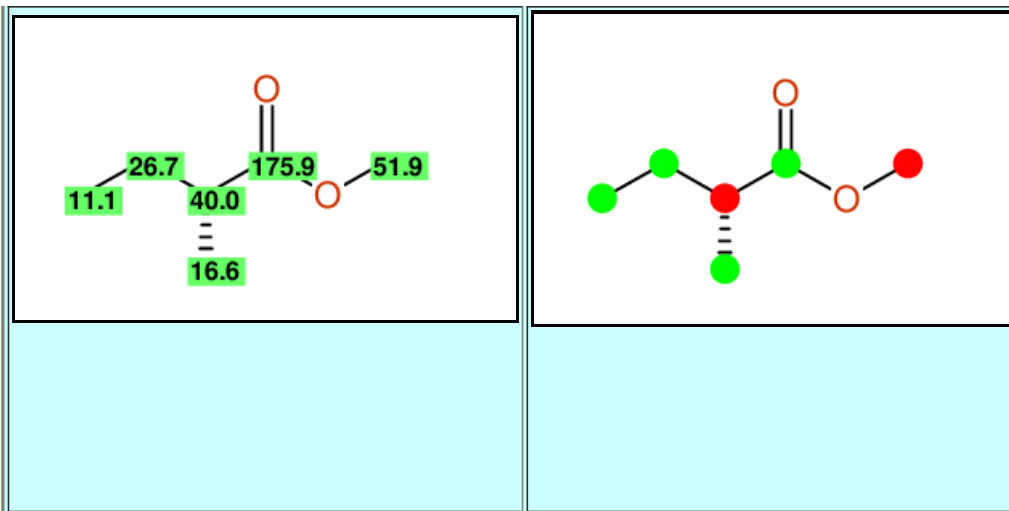
No line in reference: 



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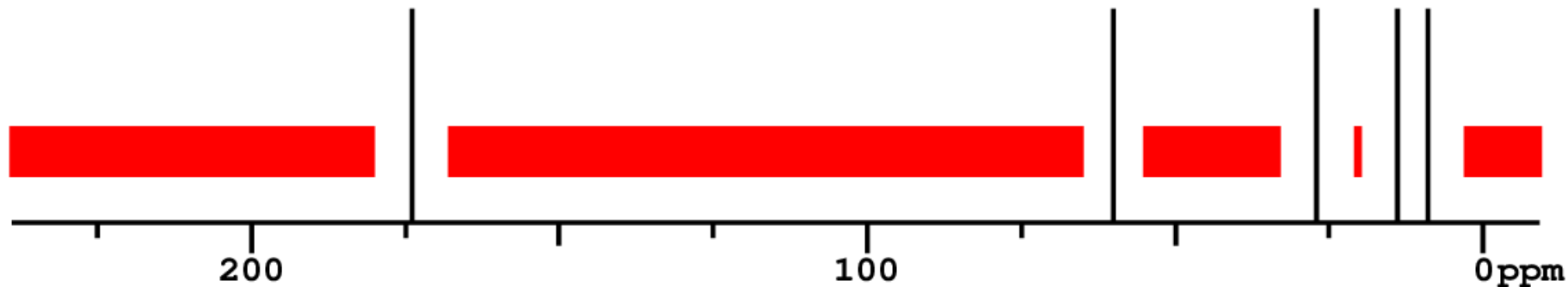
Structure Proposal #19

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 116.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>OCWLYWIFNDCWRZ</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



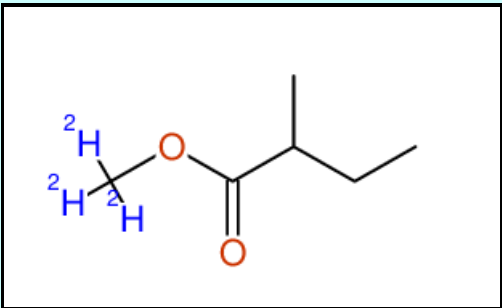
Experimental shift values

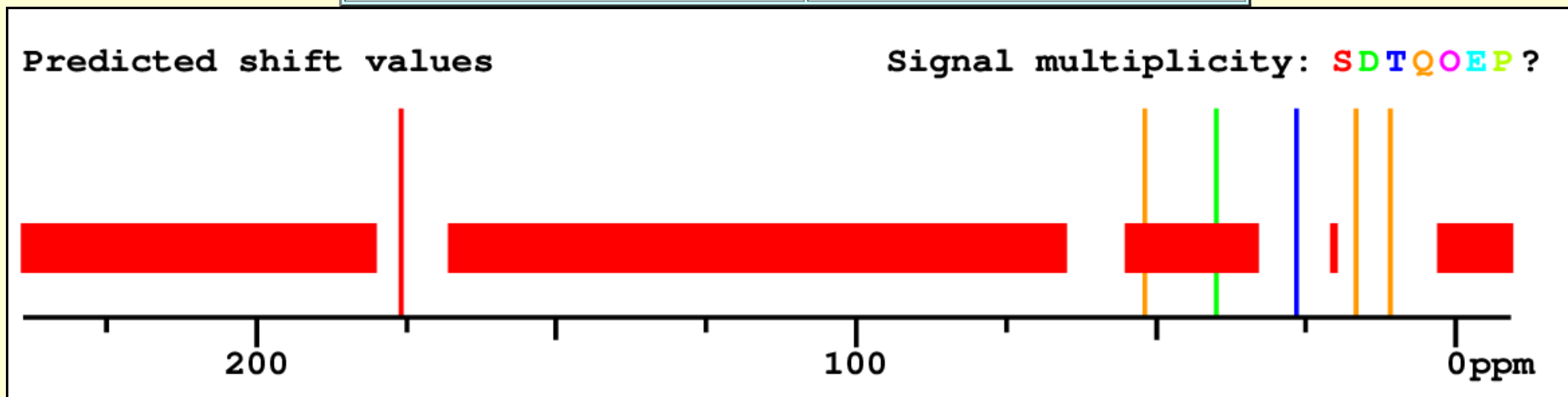
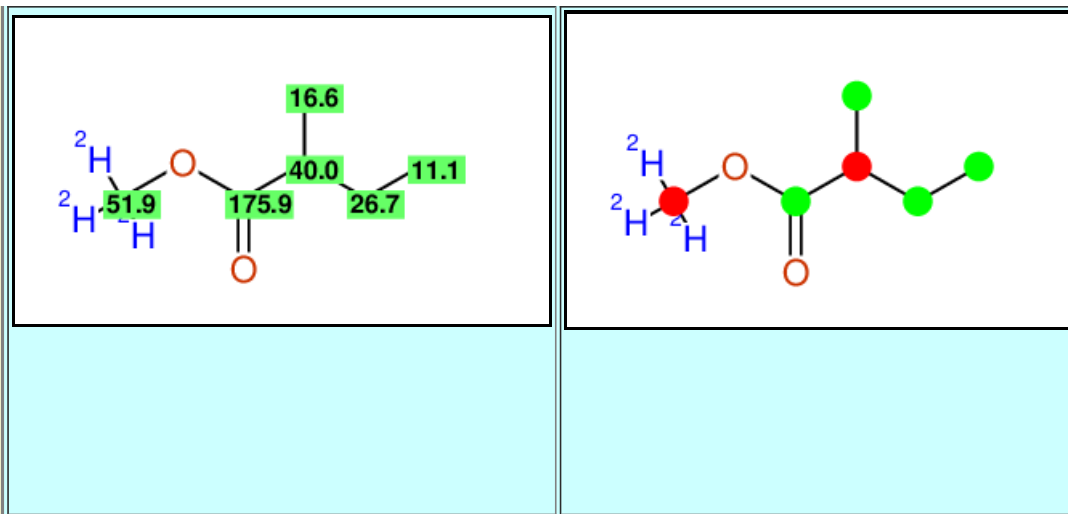
No line in reference: 



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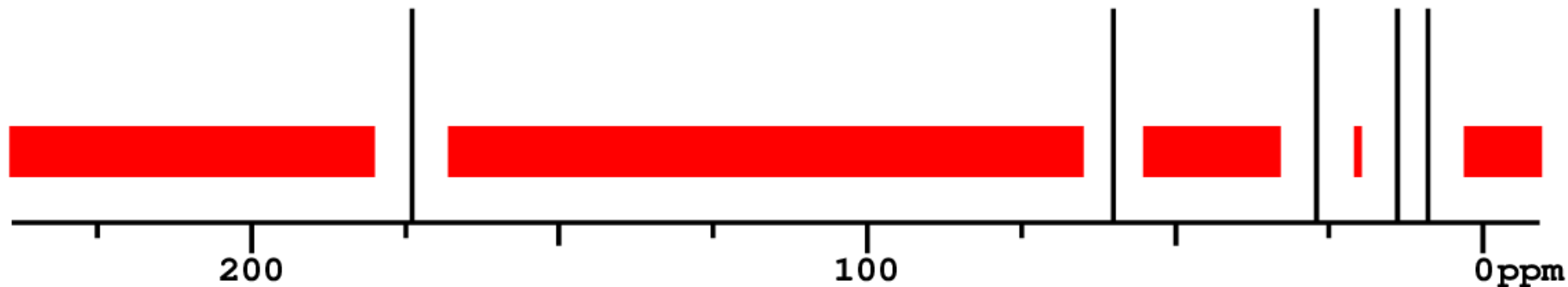
Structure Proposal #20

Structure	Similarity Measure
 <p>The chemical structure is ethyl 2-methylbutanoate. The methyl group of the ethyl part is labeled with three '2H' in blue, indicating two equivalent protons. The methylene group of the ethyl part is labeled with '2H' in blue, indicating two equivalent protons. The ester oxygen is shown in red, and the carbonyl oxygen is also shown in red.</p>	<p>Deviation = 5.25 ppm (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 119.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>OCWLYWIFNDCWRZ</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



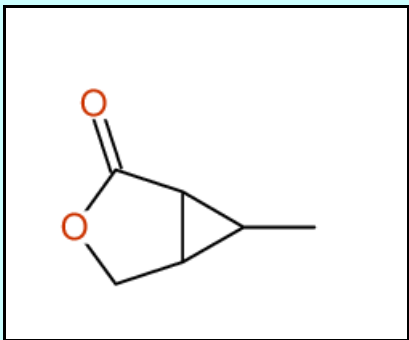
Experimental shift values

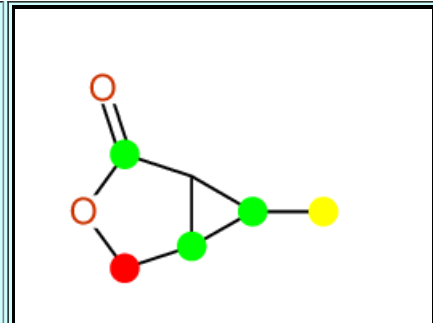
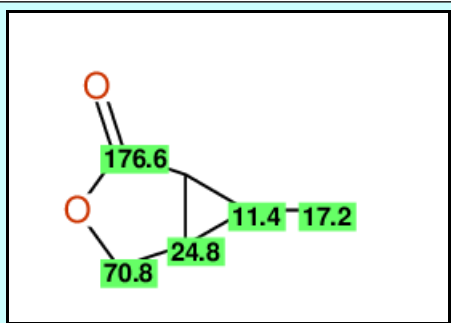
No line in reference: 



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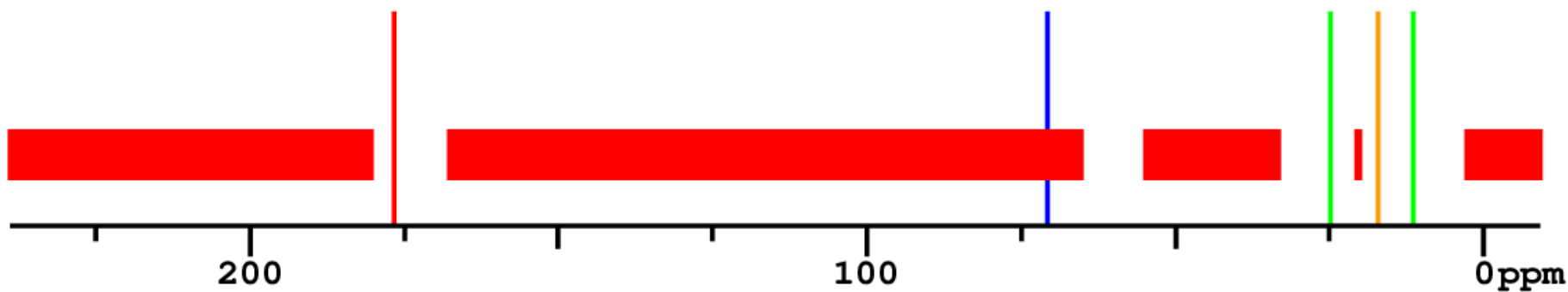
Structure Proposal #21

Structure	Similarity Measure
	<p>Deviation = 5.38 ppm (Different pattern)</p> <p>$C_6H_8O_2$</p> <p>MWT = 112.07</p> <p>PUBCHEM</p> <p>Search Web for this structure: ODZSNSOKRZBPDY</p>
Predicted Chemical Shiftvalues	Matching Map



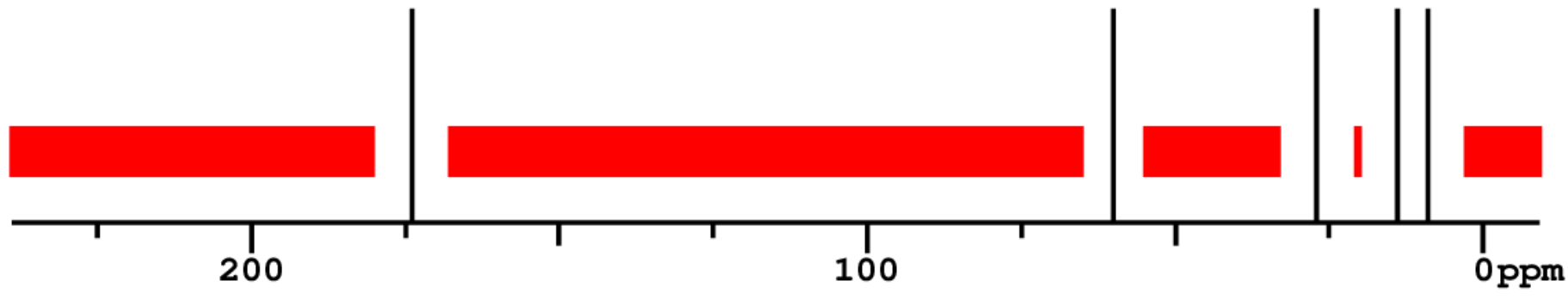
Predicted shift values

Signal multiplicity: S D T Q O E P ?



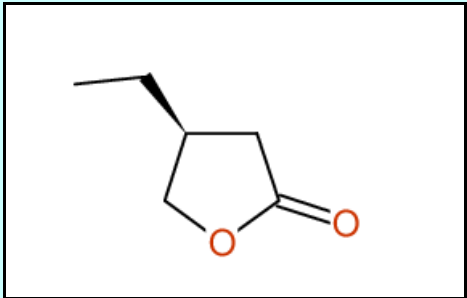
Experimental shift values

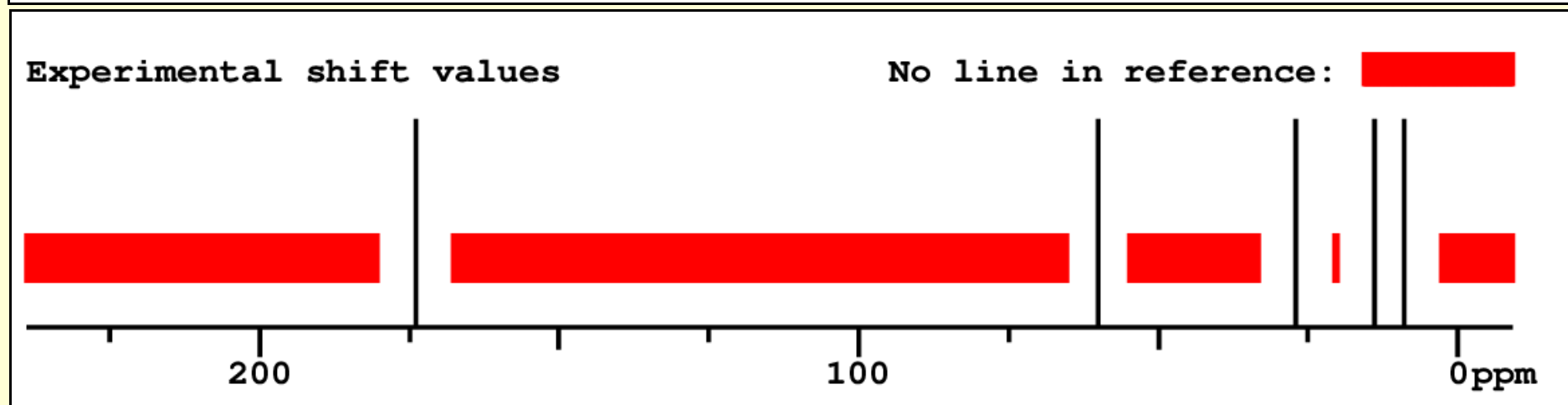
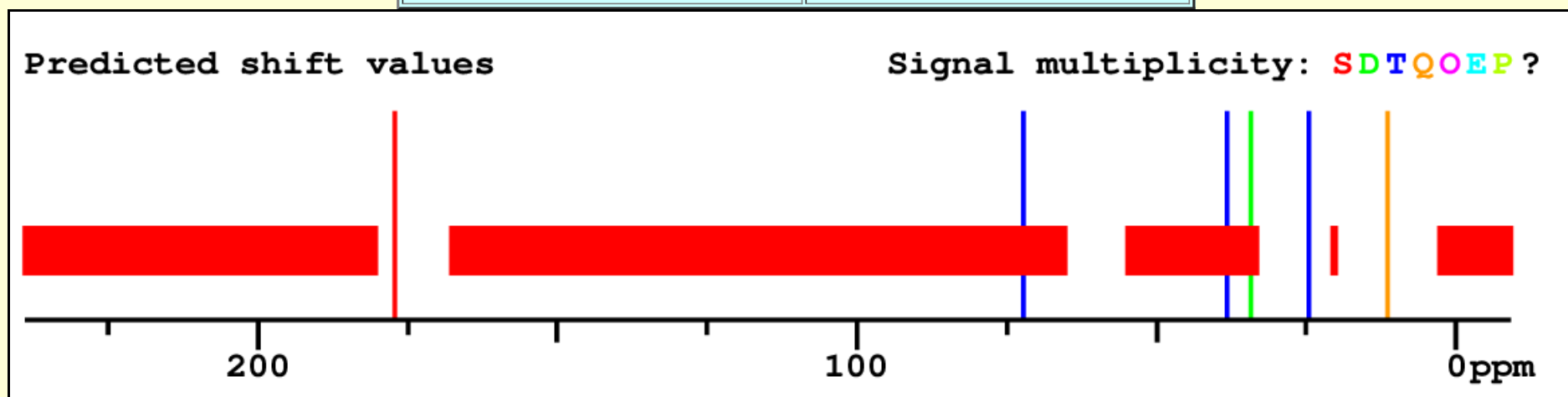
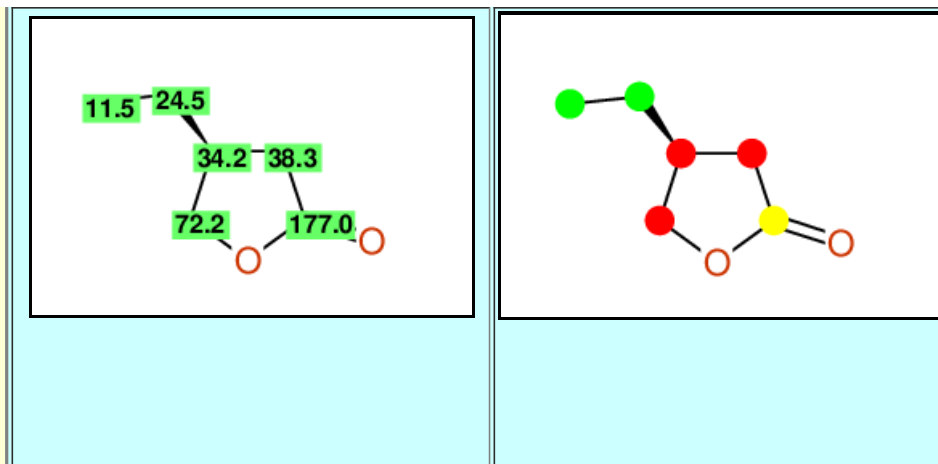
No line in reference: 



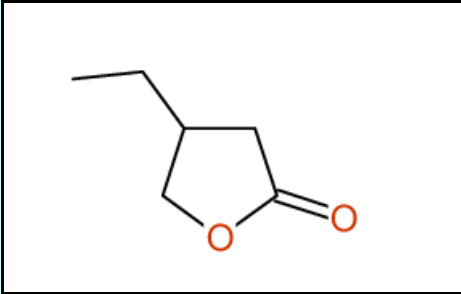
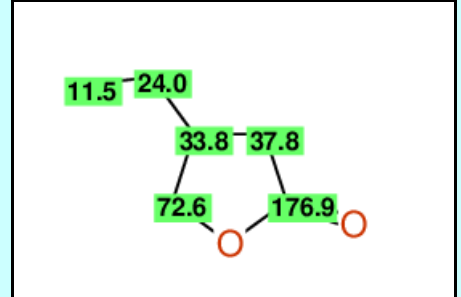
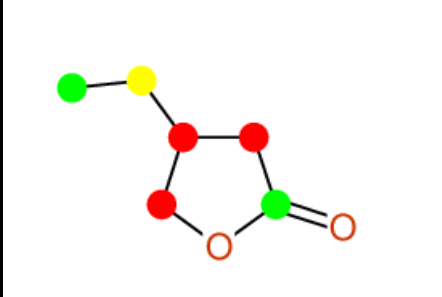
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Structure Proposal #22

Structure	Similarity Measure
	<p>Deviation = 6.77 ppm (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>MDQZVJSUBKPTHG</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map

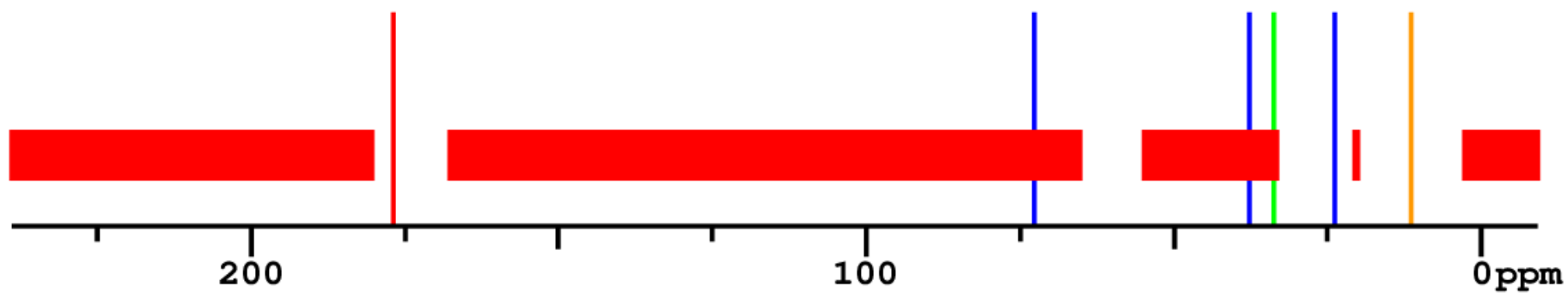


Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 6.88 ppm (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>PUBCHEM</p> <p>Search Web for this structure: MDQZVJSUBKPTHG</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map
	

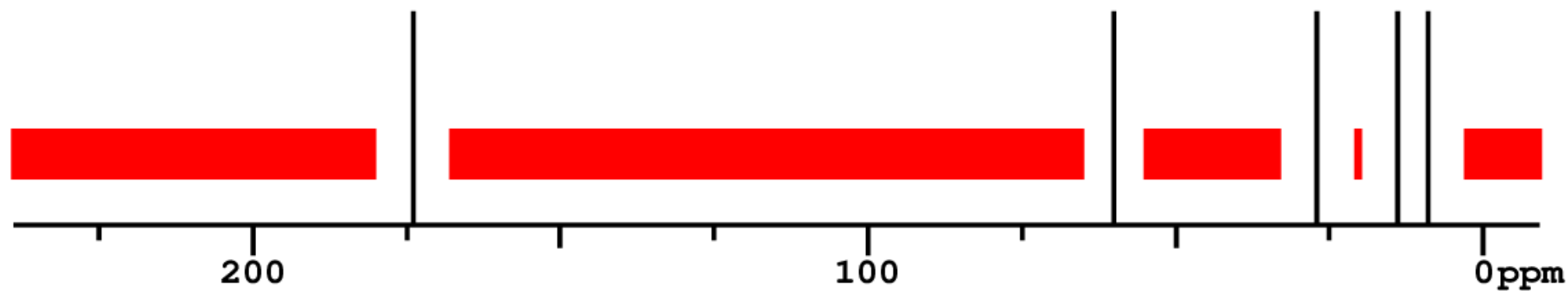
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

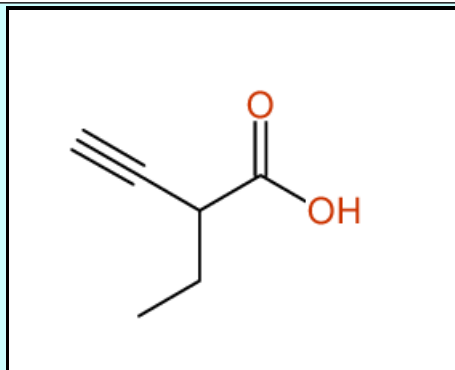
No line in reference: [red bar]



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Structure Proposal #24

Structure	Similarity Measure



Deviation = 8.49 ppm
(Different pattern)

$C_6H_8O_2$

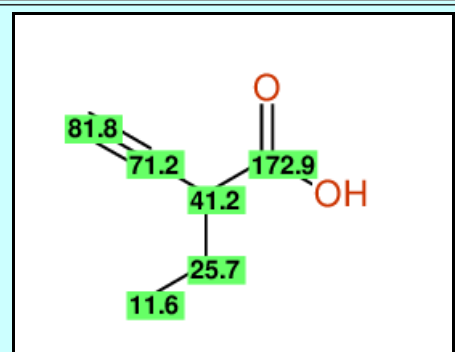
MWT = 112.07

[PUBCHEM](#)

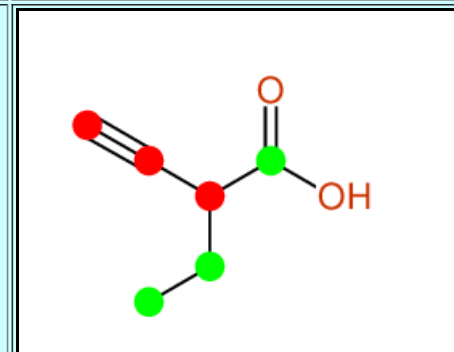
Search Web for this structure:

[YHXLBJJLZTWBAZ](#)

Predicted Chemical
Shiftvalues

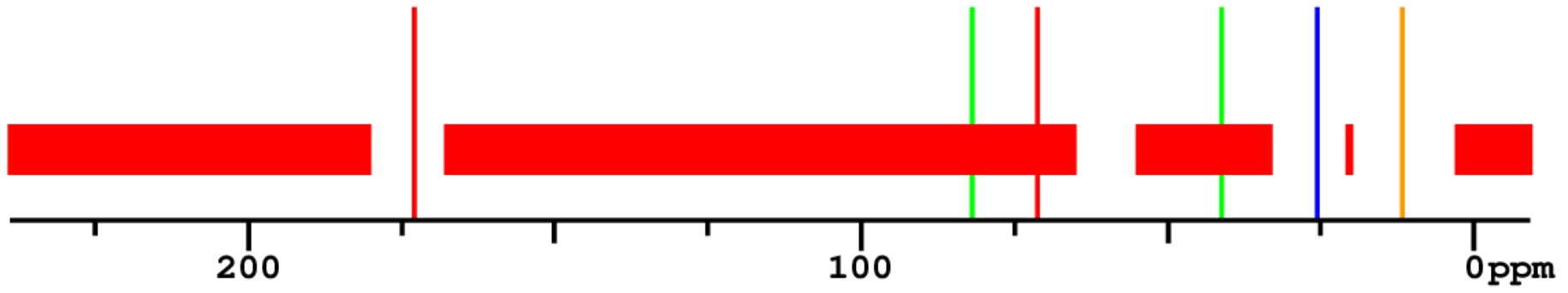


Matching Map



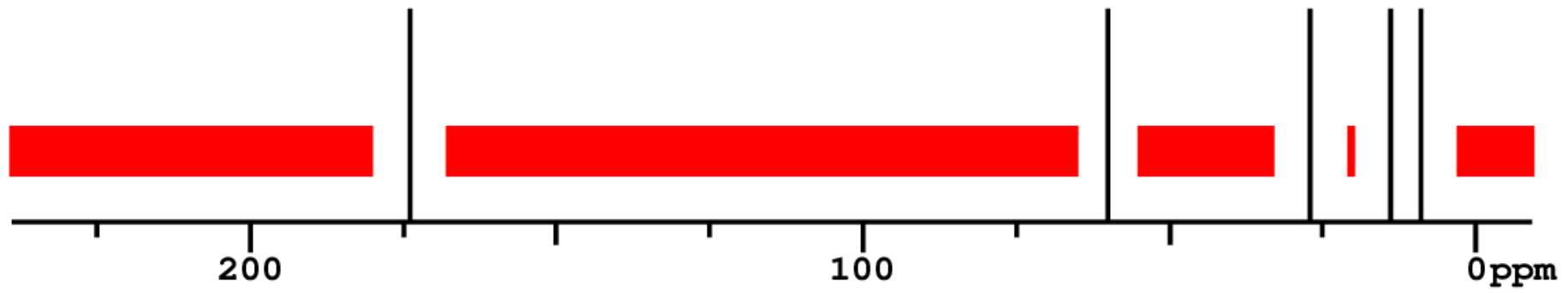
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

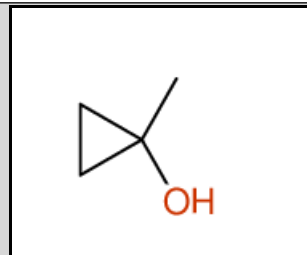


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Summary of the 1 most frequently occurring parent ring systems
within the 13 best-fitting entries

Occurrence:

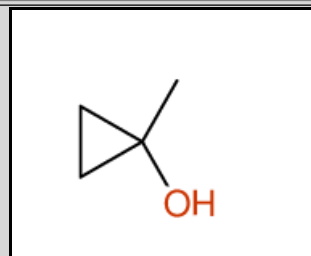
1 in 13



Summary of the 3 most frequently occurring parent ring systems
within the 21 best-fitting entries

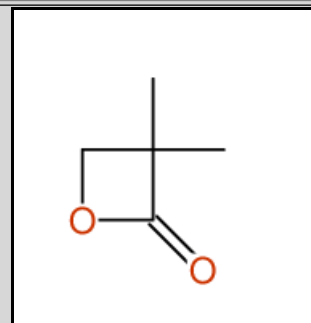
Occurrence:

1 in 21



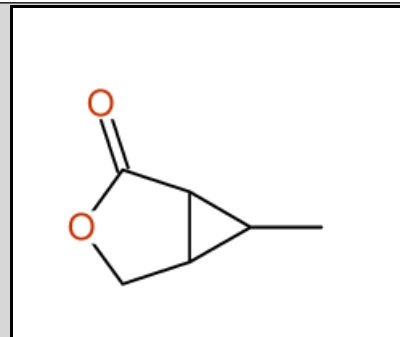
Occurrence:

1 in 21



Occurrence:

1 in 21



Summary of Processing

Checking existence of data and counting them:	74,435,185 entries in 0.210 seconds
Applying restraints from elemental composition:	1.973 seconds, 2,773,229 entries remain
Applying restraints from number of signals:	1.943 seconds, 170,467 entries remain
Searching 1,444,403,916 chemical shift values line-per-line:	20.360 seconds
Best 2,000 entries selected for analysis:	2.619 seconds
Ranking of 2,000 entries by similarity:	0.464 seconds
Deviation of best match:	0.87 ppm
Creating table and linking 2,000 structures to 475,803 INCHIKEY-pages:	0.919 seconds
Detailed Analysis of 24 structures including graphical representation:	12.999 seconds
Analysis of 21 structures for common parent ring systems	0.003 seconds
Data transfered from disk:	421 MBytes out of 272,265 MBytes
Program version:	20200916_2-3D-zip/00
Machine:	I9-9900K / 16x3.60GHz

Page written by Wolfgang Robien using CSEARCH-Technology

Page written on 2021:05:19 at 19:08

Page finished on 2021:05:19 at 19:10

Have a nice day !