

**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>

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:07

This page will be kept for 30 days here

Name of Project:

Test1

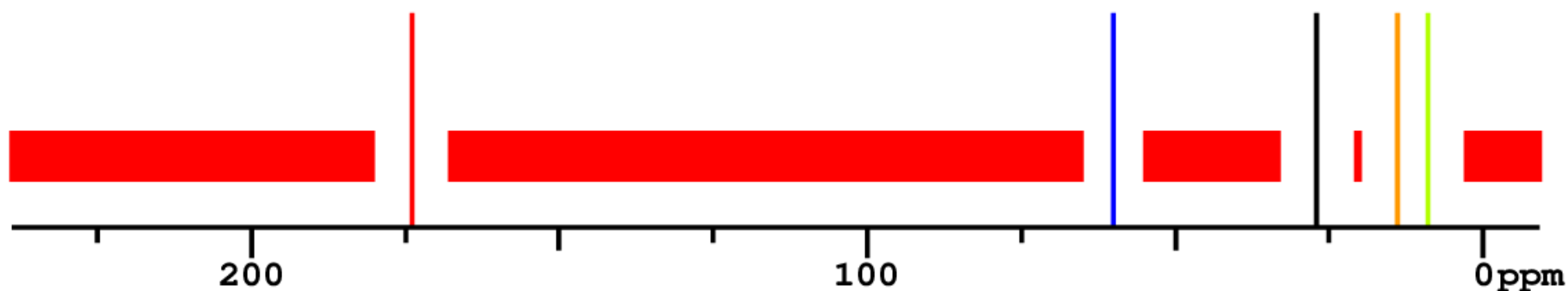
Comment:	Dereplication-engine
Name of Compound:	Propionic_acid,ethylester 400MHz

Summary of Supplied Data

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

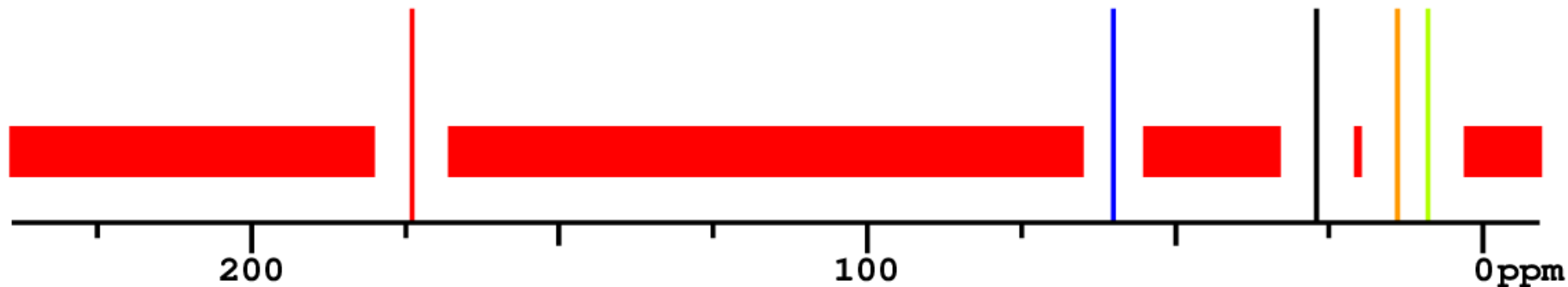
Available entries at each Screening-Step	
Total number of entries:	74,435,185

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	S	3.00	29,767	Unspecific line
2	60.00	T	2.50	22,471	Unspecific line
3	27.00	?	3.00	66,806	Unspecific line
4	14.00	Q	3.00	35,543	Unspecific line
5	9.00	P	3.00	21,626	Unspecific line

Experimental shift values

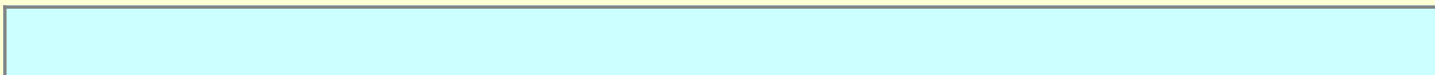
No line in reference: ██████████



Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	129	Selected for detailed analysis
4	1,433	Selected for detailed analysis
3	8,837	
2	35,013	
1	73,299	

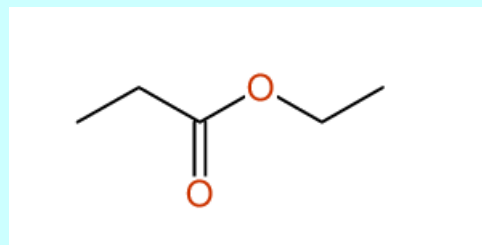
Best 20 Proposals shown for Compound: Propionic_acid,ethylester::400MHz



0.87 -
0.87ppm

3x found

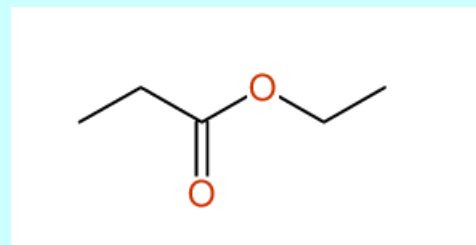
[FKRCODPIKNYEAC](#)



0.87 -
0.87ppm

1x found

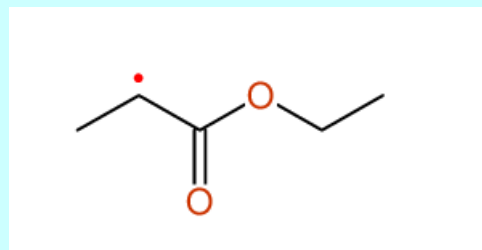
[BYLOWUCDFUYIQ](#)



0.87 -
0.87ppm

1x found

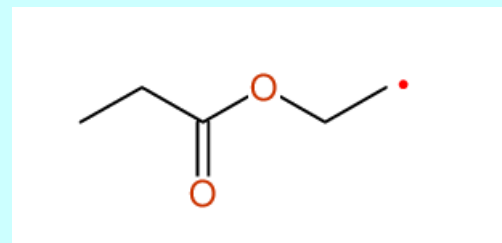
[UPRLWNPAOPKPCE](#)



0.87 -
0.87ppm

1x found

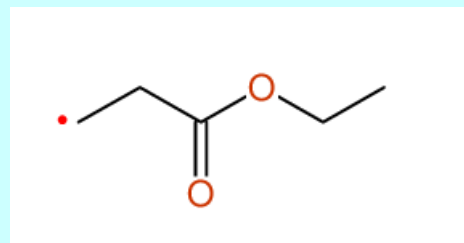
[IRGLFRDZYNBBCO](#)



0.87 -
0.87ppm

1x found

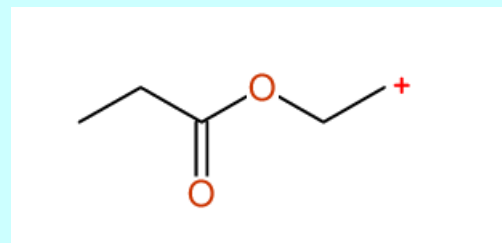
[SQKCNILPAQLIRC](#)



0.87 -
0.87ppm

1x found

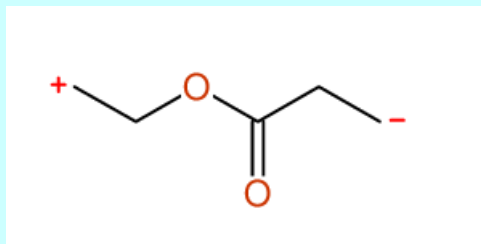
[GOKITYWXYBHPKU](#)



0.87 -
0.87ppm

1x found

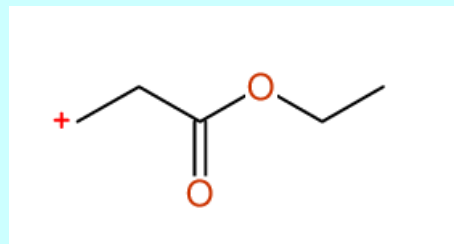
[LVCAAHDUTLIBML](#)



0.87 -
0.87ppm

1x found

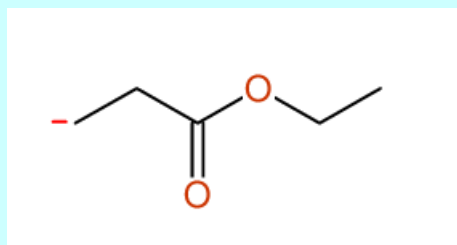
[MUQMZQYQIIBIT](#)



0.87 -
0.87ppm

1x found

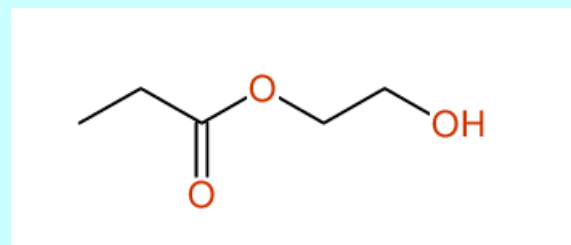
[NWIUUTFORIXPJC](#)



2.02 -
2.02ppm

1x found

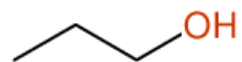
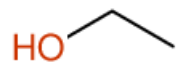
[SFAMKDPMPDEXGH](#)



2.62 -
2.62ppm

1x found

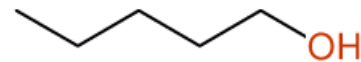
[OMRDZQXXMYCHBU](#)



2.98 -
2.98ppm

1x found

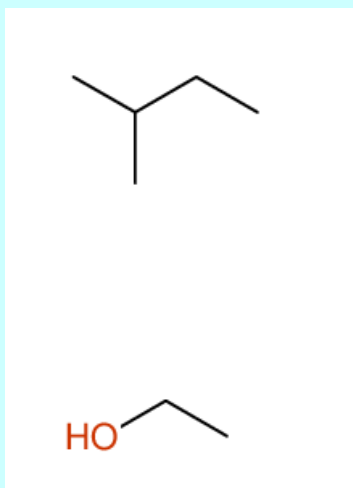
[ZARMDFHJSJSIZKQ](#)



3.16 -
3.16ppm

1x found

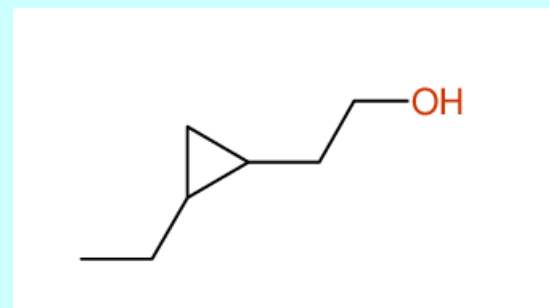
FOXQTCHXXJKLNK



3.49 -
3.49ppm

1x found

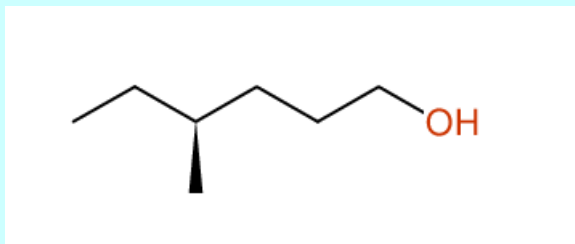
IPKMDCPNAOYUEB



4.01 -
4.01ppm

3x found

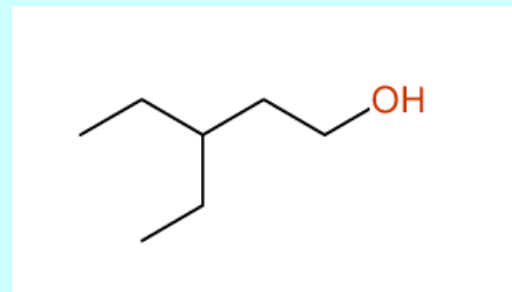
[YNPVLWKVZZBTM](#)



4.36 -
4.36ppm

1x found

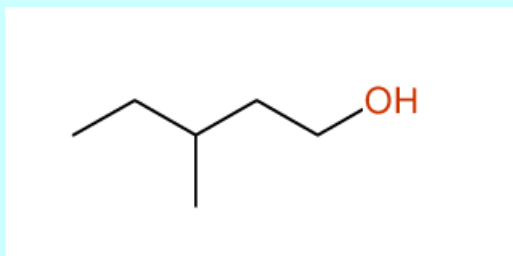
[DVEFUHVWJONKR](#)



4.64 -
4.64ppm

3x found

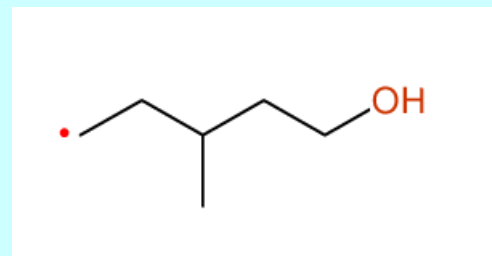
[IWTBVKIGCDZRPL](#)



4.64 -
4.64ppm

1x found

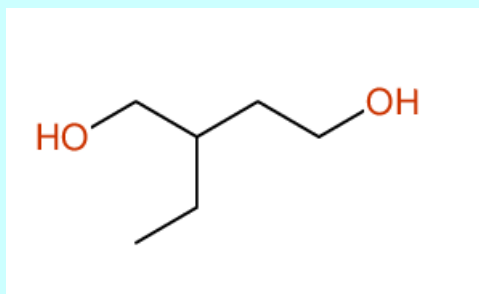
[FCACGIMTGMLTKJ](#)



4.98 -
4.98ppm

3x found

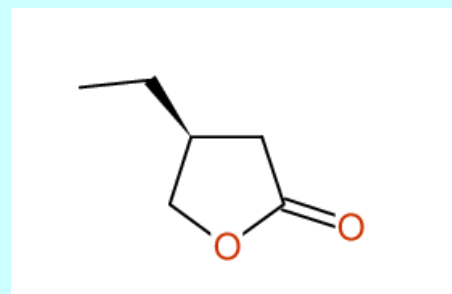
[CYVMBANVYOZFIG](#)



6.77 -
6.88ppm

2x found

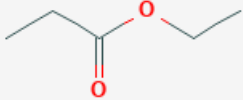

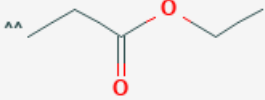
[MDQZVJSUBKPTHG](#)

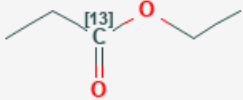

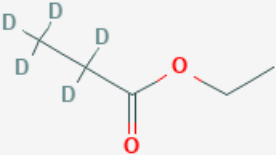



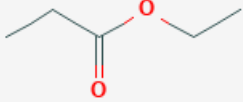
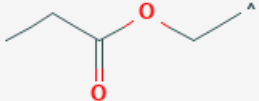
1,562 [Structure proposals](#) found for your C-NMR Spectrum

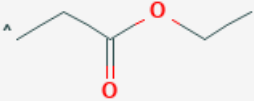
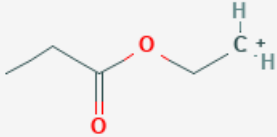
50 Entries will be shown because of your selection of additional constraints

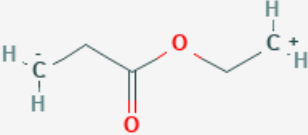
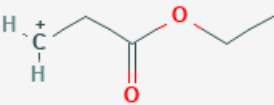
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼

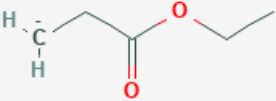
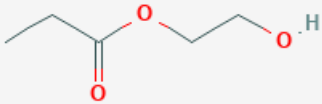
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 102.055</p>	<p>Proposal #1</p> <p>FKRCODPIKNYEAC-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 7749</p>	<p>Availability of NMR-Data in 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 ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 103.055</p>	<p>Proposal #3</p> <p>FKRCODPIKNYEAC-HOSYLAQJSA-N</p> <p>PUBCHEM Compound: 12229103</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 107.055</p>	<p>Proposal #4</p> <p>FKRCODPIKNYEAC-WNWXORZSA-N</p> <p>PUBCHEM Compound: 89254459</p>	<p>Availability of NMR-Data in CSEARCH</p> 

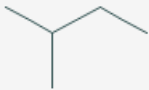

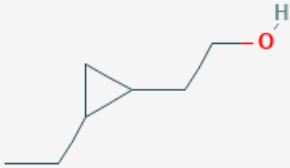

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>C₅H₉O₂</p> <p>MWT = 101.055</p>	<p>Proposal #5</p> <p>UPRLWNPAOPKPCE-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 5371171</p>	
<p>0.87</p> <p>Details</p>		<p>C₅H₉O₂</p> <p>MWT = 101.055</p>	<p>Proposal #6</p> <p>IRGLFRDZYNBBCO-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57419189</p>	

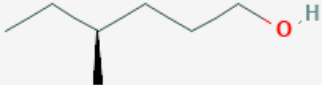

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_9O_2$</p> <p>MWT = 101.055</p>	<p>Proposal #7</p> <p>SQKCNILPACLIRC-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12568583</p>	
<p>0.87</p> <p>Details</p>		<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>	

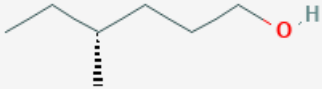

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>		<p>$C_5H_8O_2$</p> <p>MWT = 100.055</p>	<p>Proposal #9</p> <p>LVCAAHDUTLIBML-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 53630283</p>	
<p>0.87</p> <p>Details</p>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

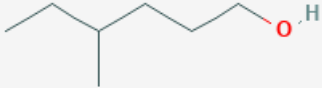

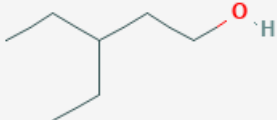

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>0.87</p> <p>Details</p>	 <p>The structure shows a propyl chain (CH₂-CH₂-CH₃) attached to a carbonyl group (C=O), which is further bonded to an ethyl group (CH₂-CH₃) via an oxygen atom. The carbonyl oxygen is shown in red.</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>	
<p>2.02</p> <p>Details</p>	 <p>The structure shows a propyl chain (CH₂-CH₂-CH₃) attached to a carbonyl group (C=O), which is further bonded to another propyl chain (CH₂-CH₂-CH₃) via an oxygen atom. The carbonyl oxygen is shown in red.</p>	<p>$C_5H_{10}O_3$</p> <p>MWT = 118.055</p>	<p>Proposal #12</p> <p>SFAMKDPMPDEXGH-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 545098</p>	

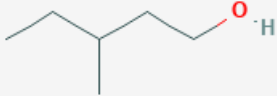

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>2.62</p> <p>Details</p>	 	<p>$C_5H_{14}O_2$</p> <p>MWT = 106.055</p>	<p>Proposal #13</p> <p>OMRDZQXXMYCHBU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 9793718</p>	
<p>2.98</p> <p>Details</p>	 	<p>$C_7H_{18}O$</p> <p>MWT = 118.077</p>	<p>Proposal #14</p> <p>ZARMDFHSJSIZKQ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 54537300</p>	

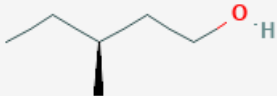

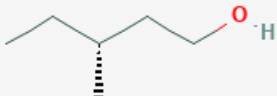

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>3.16</p> <p>Details</p>	 	<p>$C_7H_{18}O$</p> <p>MWT = 118.077</p>	<p>Proposal #15</p> <p>FOXQTCHXXJKLNK-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 21646453</p>	
<p>3.49</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #16</p> <p>IPKMDCPNAOYUEB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 23329956</p>	<p>Availability of NMR-Data in CSEARCH</p> 

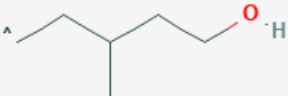
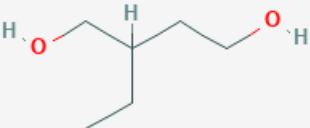
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.01 Details Different pattern	 <p>The diagram shows the skeletal structure of 2-methyl-1-pentanol. It consists of a five-carbon chain with a methyl group attached to the second carbon and a hydroxyl group (-OH) attached to the first carbon. The hydroxyl group is shown in red with a white hydrogen atom.</p>	C ₇ H ₁₆ O MWT = 116.077	Proposal #17 YNPVNLWKVZZBTM-ZETCQYMHSA-N PUBCHEM Compound: 13463446	Availability of NMR-Data in CSEARCH 

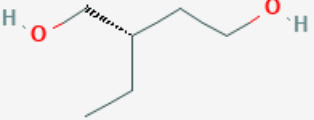
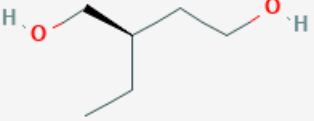
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.01 Details Different pattern	 <p>The diagram shows the skeletal structure of 1-methyl-1-hexanol. It consists of a six-carbon main chain with a methyl group attached to the first carbon. The first carbon is also bonded to a hydroxyl group (-OH). The methyl group is shown with a dashed bond, indicating it is pointing away from the viewer.</p>	$C_7H_{16}O$ MWT = 116.077	Proposal #18 YNPVNLWKVZZBTM-SSDOTTSWSA-N PUBCHEM Compound: 13463447	Availability of NMR-Data in CSEARCH 

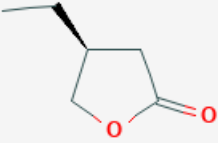

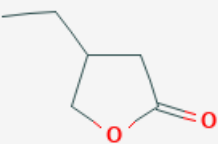

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>4.01</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #19</p> <p>YNPVNLWKVZZBTM-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 98346</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>4.36</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #20</p> <p>DVEFUHVWVWJONKR-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 641005</p>	<p>Availability of NMR-Data in CSEARCH</p> 

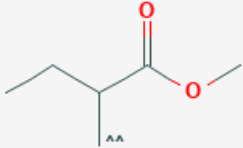
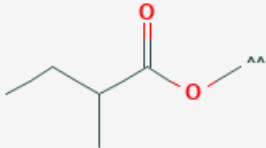
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p data-bbox="197 576 255 600">4.64</p> <p data-bbox="176 639 271 663">Details</p> <p data-bbox="125 700 327 724">Different pattern</p>	 <p>The image shows the skeletal structure of 2-methyl-1-butanol, a six-carbon primary alcohol with a methyl branch on the second carbon.</p>	<p data-bbox="1037 544 1133 568">$C_6H_{14}O$</p> <p data-bbox="992 608 1178 632">MWT = 102.066</p>	<p data-bbox="1458 501 1621 525">Proposal #21</p> <p data-bbox="1312 592 1756 616">IWTBVKIGCDZRPL-UHFFFAOYSA-N</p> <p data-bbox="1357 652 1720 676">PUBCHEM Compound: 11508</p>	<p data-bbox="1906 312 2069 392">Availability of NMR-Data in CSEARCH</p>  <p>A square QR code is centered in the cell, likely linking to the NMR data mentioned in the text above it.</p>

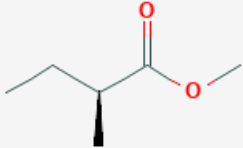

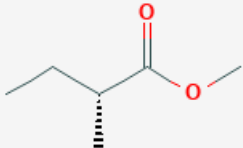

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>4.64</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #22</p> <p>IWTBVKIGCDZRPL-LURJTMIESA-N</p> <p>PUBCHEM Compound: 641003</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>4.64</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #23</p> <p>IWTBVKIGCDZRPL-ZCFIWIBFSA-N</p> <p>PUBCHEM Compound: 6999792</p>	<p>Availability of NMR-Data in CSEARCH</p> 

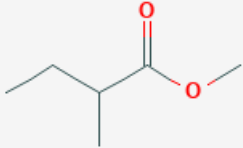

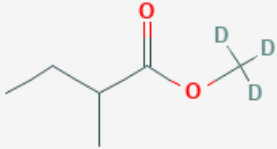

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>4.64</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a three-carbon chain with a methyl group on the second carbon and a hydroxyl group on the first carbon.</p>	<p>$C_6H_{13}O$</p> <p>MWT = 101.066</p>	<p>Proposal #24</p> <p>FCACGIMTGMLTKJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57432776</p>	
<p>4.98</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a central carbon atom bonded to a hydrogen atom, an ethyl group, and two hydroxymethyl groups.</p>	<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #25</p> <p>CYVMBANVYOZFIG-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12648201</p>	

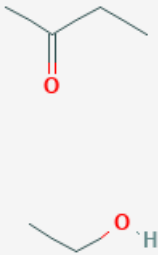
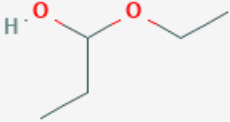

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>4.98</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a four-carbon chain with a hydroxyl group (-OH) attached to the second carbon. The hydroxyl group is shown with a dashed bond, indicating it is on the opposite side of the plane from the viewer.</p>	<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #26</p> <p>CYMBANVYOZFIG-LURJTMIESA-N</p> <p>PUBCHEM Compound: 12648202</p>	
<p>4.98</p> <p>Details</p> <p>Different pattern</p>	 <p>The structure shows a four-carbon chain with a hydroxyl group (-OH) attached to the second carbon. The hydroxyl group is shown with a solid wedge bond, indicating it is on the same side of the plane as the viewer.</p>	<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #27</p> <p>CYMBANVYOZFIG-ZCFIWIBFSA-N</p> <p>PUBCHEM Compound: 11804732</p>	

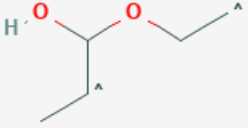
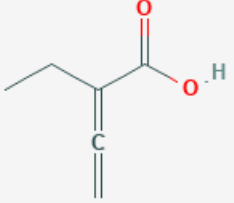
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>6.77</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #28</p> <p>MDQZVJSUBKPTHG-YFKPBYSVSA-N</p> <p>PUBCHEM Compound: 57939696</p>	<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 #29</p> <p>MDQZVJSUBKPTHG-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 27893</p>	<p>Availability of NMR-Data in CSEARCH</p> 

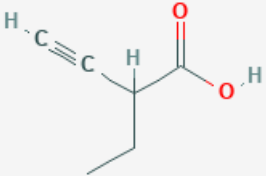
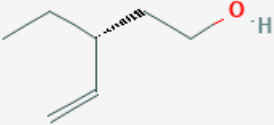
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>13.29</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #30</p> <p>YMRCZGBILKTSCL-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 59258212</p>	
<p>13.29</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #31</p> <p>OYGDMLWOJBKWLN-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 59990131</p>	

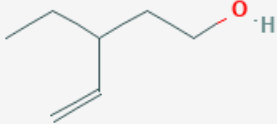
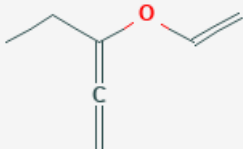

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>13.29</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #32</p> <p>OCWLYWIFNDCWRZ-YFKPBYRVSA-N</p> <p>PUBCHEM Compound: 643001</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>13.29</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #33</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>13.29</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #34</p> <p>OCWLYWIFNDCWRZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 13357</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>13.29</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 119.066</p>	<p>Proposal #35</p> <p>OCWLYWIFNDCWRZ-HPRDVNIFSA-N</p> <p>PUBCHEM Compound: 60069722</p>	<p>Availability of NMR-Data in CSEARCH</p> 



Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>15.10</p> <p>Different pattern</p>	 <p>The diagram shows two chemical structures. The top structure is 2-butanone (CH₃CH₂COCH₃), a four-carbon chain with a carbonyl group at the second position. The bottom structure is ethanol (CH₃CH₂OH), a two-carbon chain with a hydroxyl group at the end.</p>	<p>C₆H₁₄O₂</p> <p>MWT = 118.066</p>	<p>Proposal #36</p> <p>CASOXAYOCHCWQU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 22558530</p>	
<p>17.85</p> <p>Different pattern</p>	 <p>The diagram shows the chemical structure of 2-ethoxybutane (CH₃CH₂CH(OH)CH₂CH₃), a four-carbon chain with a hydroxyl group at the second position and an ethoxy group (-OCH₂CH₃) also at the second position.</p>	<p>C₅H₁₂O₂</p> <p>MWT = 104.055</p>	<p>Proposal #37</p> <p>JLBXCKSMESLGTJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 93269</p>	<p>Availability of NMR-Data in CSEARCH</p> 

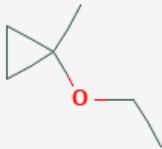
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>17.85</p> <p>Different pattern</p>	 <p>Chemical structure of ethyl propyl ether (C₅H₁₀O₂).</p>	<p>C₅H₁₀O₂</p> <p>MWT = 102.055</p>	<p>Proposal #38</p> <p>VOXZYDHLZQKQCB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 90787265</p>	
<p>19.52</p> <p>Different pattern</p>	 <p>Chemical structure of 2-methylbut-2-enoic acid (C₆H₈O₂).</p>	<p>C₆H₈O₂</p> <p>MWT = 112.066</p>	<p>Proposal #39</p> <p>PSBUQOAVEMYGEF-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 15570377</p>	

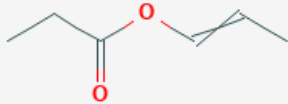
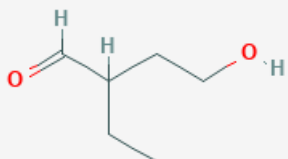
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>22.42</p> <p>Different pattern</p>		<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #40</p> <p>YHXLBJJLZTWBAZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12491392</p>	
<p>26.40</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #41</p> <p>LRKICXFRWQFVSZ-SSDOTTSWSA-N</p> <p>PUBCHEM Compound: 24767552</p>	

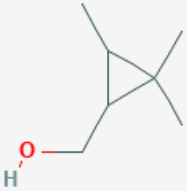
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>26.40</p> <p>Different pattern</p>		<p>$C_7H_{14}O$</p> <p>MWT = 114.077</p>	<p>Proposal #42</p> <p>LRKICXFRWQFVSZ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 86167614</p>	
<p>26.50</p> <p>Different pattern</p>		<p>$C_7H_{10}O$</p> <p>MWT = 110.077</p>	<p>Proposal #43</p> <p>MFKQNKFYXTXLMB-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 15084427</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
31.36 Different pattern		C ₇ H ₁₆ O MWT = 116.077	Proposal #44 KFRVYYGHSPLXSZ-UHFFFAOYSA-N PUBCHEM Compound: 13527	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>31.36</p> <p>Different pattern</p>	 <p>The structure shows a central carbon atom bonded to two methyl groups, one ethyl group, and one deuterated methyl group. The deuterated methyl group is labeled with three 'D' atoms.</p>	<p>C₇H₁₆O</p> <p>MWT = 119.077</p>	<p>Proposal #45</p> <p>KFRVYYGHSPLXSZ-FIBGUPNXSA-N</p> <p>PUBCHEM Compound: 10534657</p>	
<p>31.36</p> <p>Different pattern</p>	 <p>The structure shows a central carbon atom bonded to two methyl groups, one ethyl group, and one deuterated ethyl group. The deuterated ethyl group is labeled with two 'D' atoms.</p>	<p>C₇H₁₅O</p> <p>MWT = 115.077</p>	<p>Proposal #46</p> <p>NFHQDZUNLMHWRI-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 57481895</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
32.40	 <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 #47 FSYJSAIZYZZLQM-UHFFFAOYSA-N PUBCHEM Compound: 53642689	

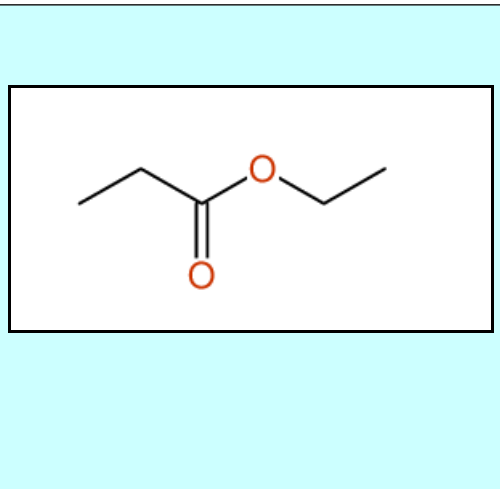
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>35.28</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #48</p> <p>AOJIRGQJECGWRU-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 53653613</p>	
<p>38.45</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #49</p> <p>CBSYYWQEKMTXTJ-UHFFFAOYSA-N</p> <p>PUBCHEM Compound: 12367599</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
38.93		<p>$C_7H_{14}O$ MWT = 114.077</p>	<p>Proposal #50 SIFLEUDKOSRPAP-UHFFFAOYSA-N PUBCHEM Compound: 14202705</p>	

Detailed Analysis

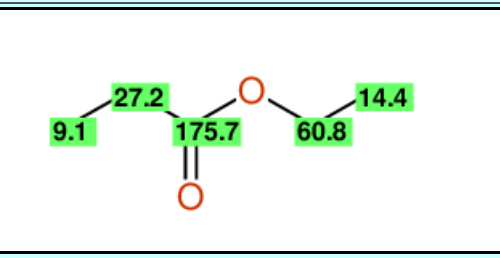
Structure Proposal #1

Structure	Similarity Measure

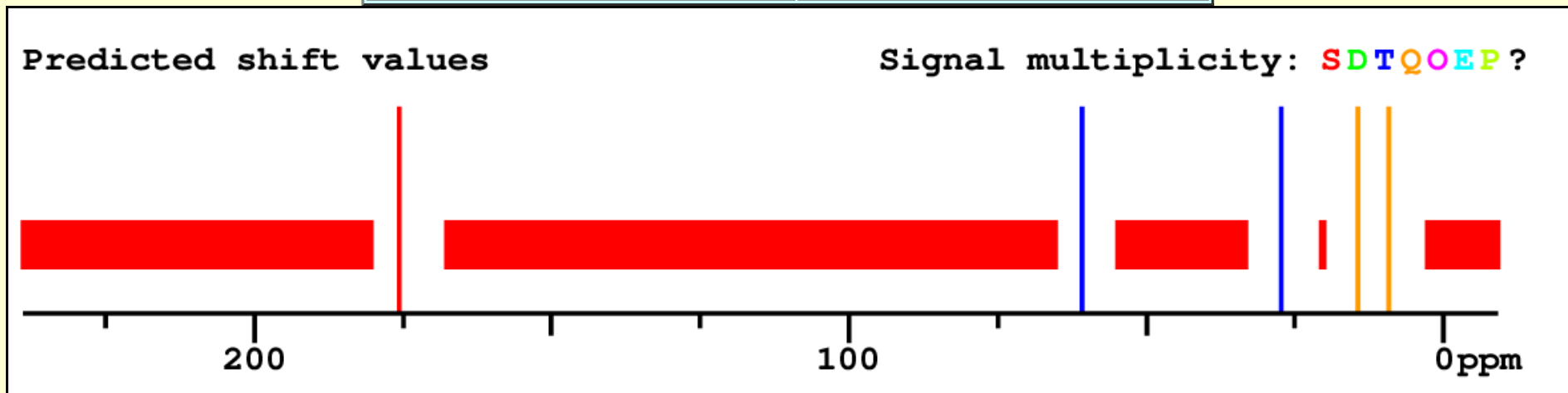
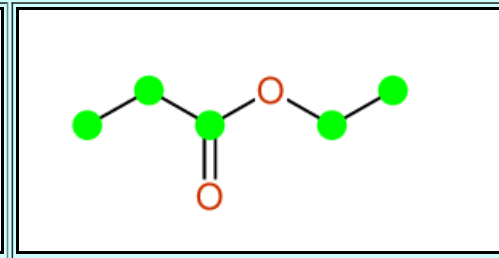


Deviation = 0.87 ppm
C₅H₁₀O₂
MWT = 102.06
[PUBCHEM](#)
Search Web for this structure:
[FKRCODPIKNYEAC](#)
[Availability](#)


Predicted Chemical Shiftvalues

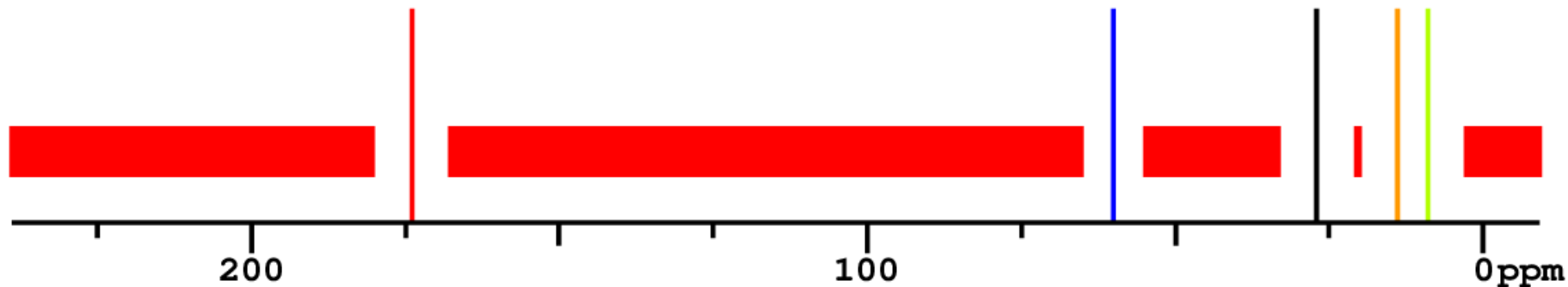


Matching Map



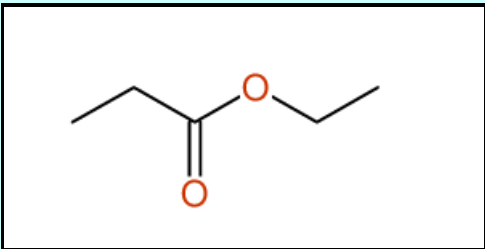
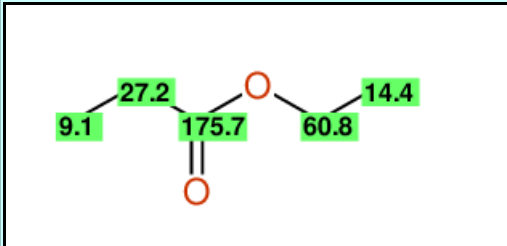
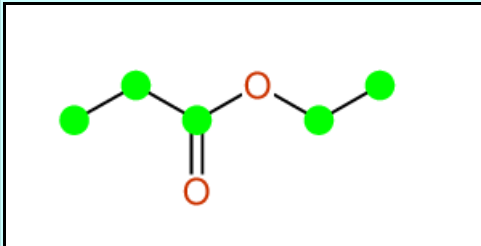
Experimental shift values

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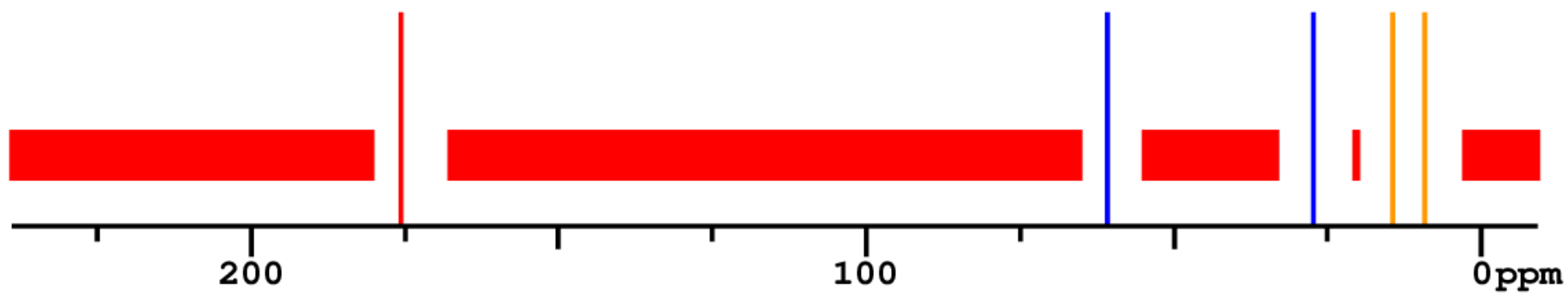
[Back to Complete Result](#)

Structure Proposal #2

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>BYLOWUCDFUYIQ</p>
Predicted Chemical Shiftvalues	Matching Map
	

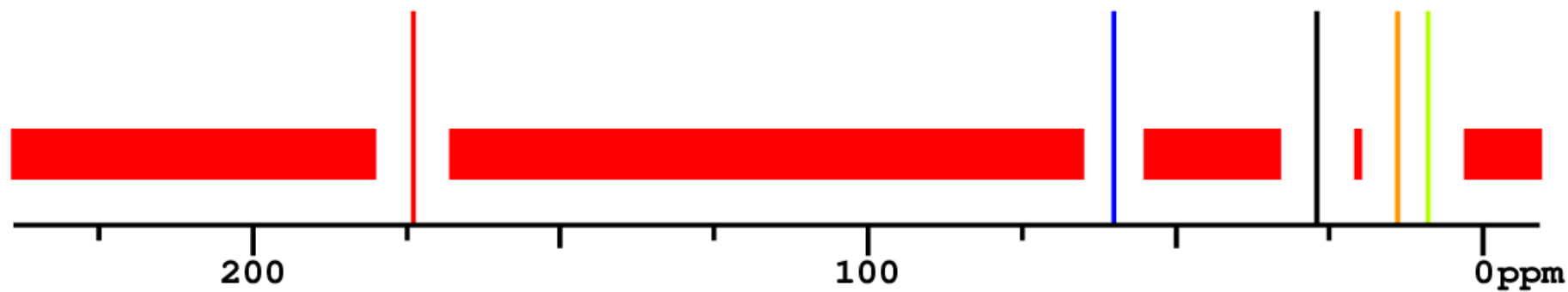
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

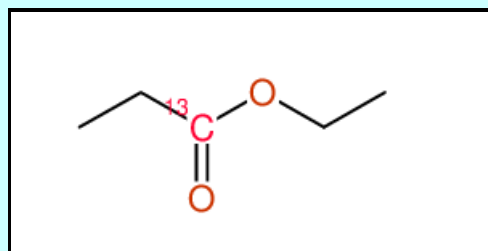
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[Back to Complete Result](#)

Structure Proposal #3

Structure	Similarity Measure



Deviation = 0.87 ppm

$\text{C}_5\text{H}_{10}\text{O}_2$

MWT = 103.06

[PUBCHEM](#)

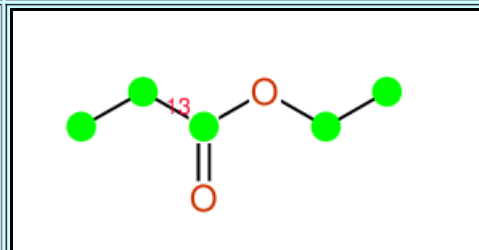
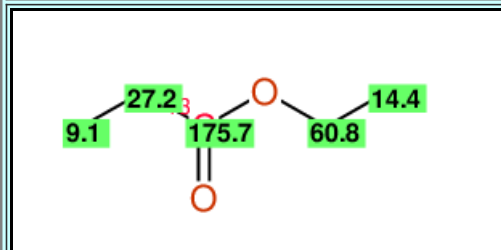
Search Web for this structure:

[FKRCODPIKNYEAC](#)

[Availability](#)

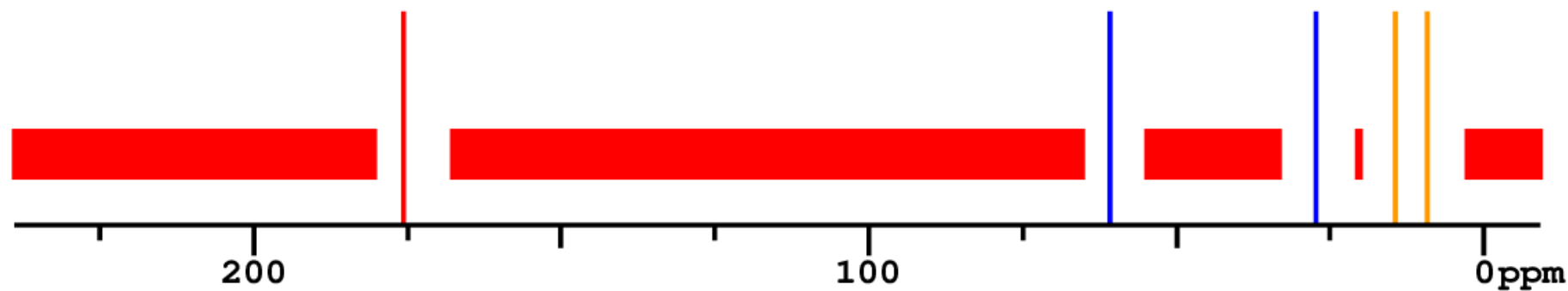
Predicted Chemical Shiftvalues

Matching Map



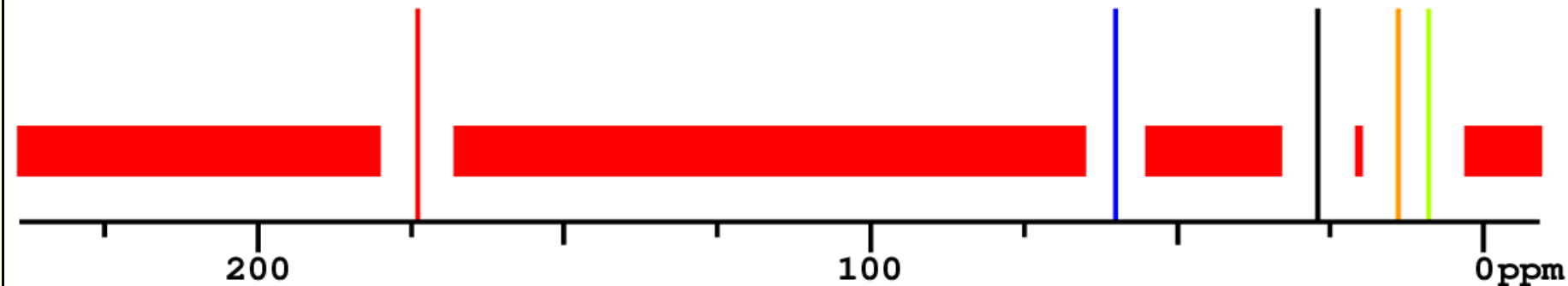
Predicted shift values

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



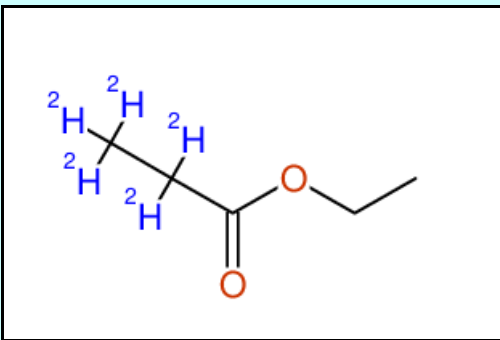
Experimental shift values

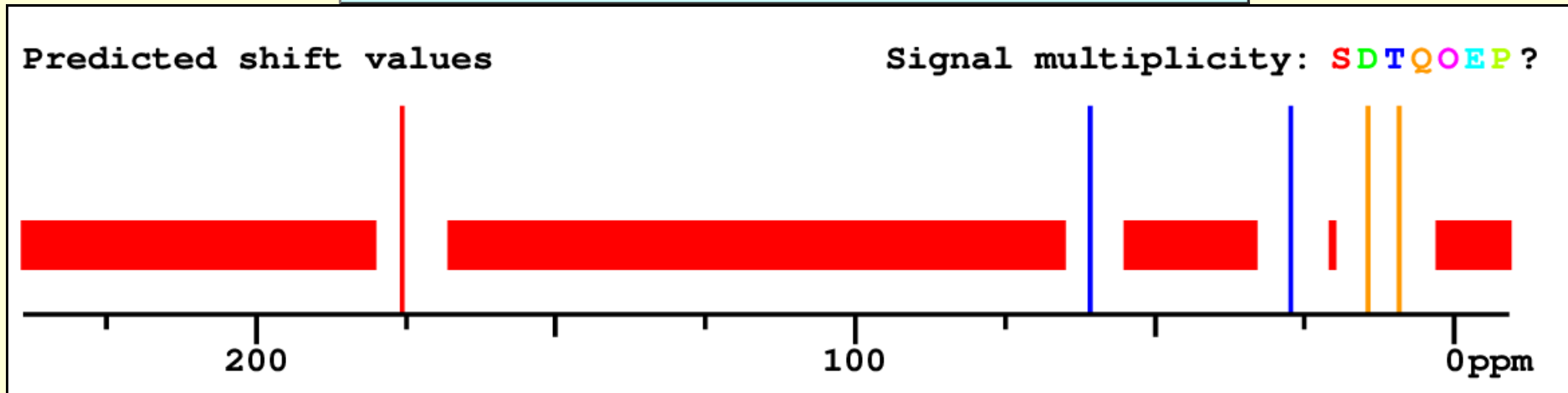
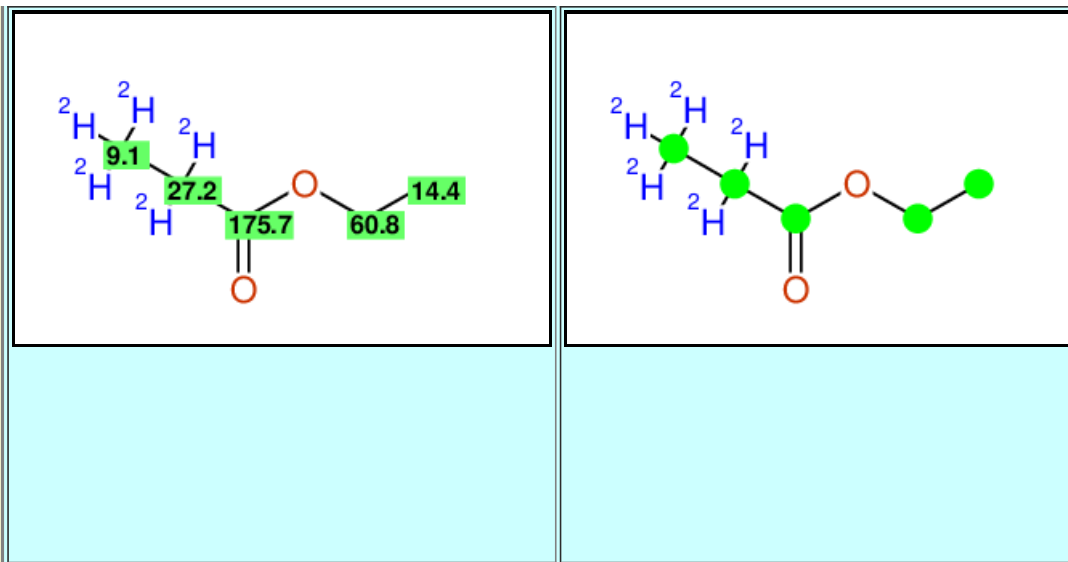
No line in reference: 



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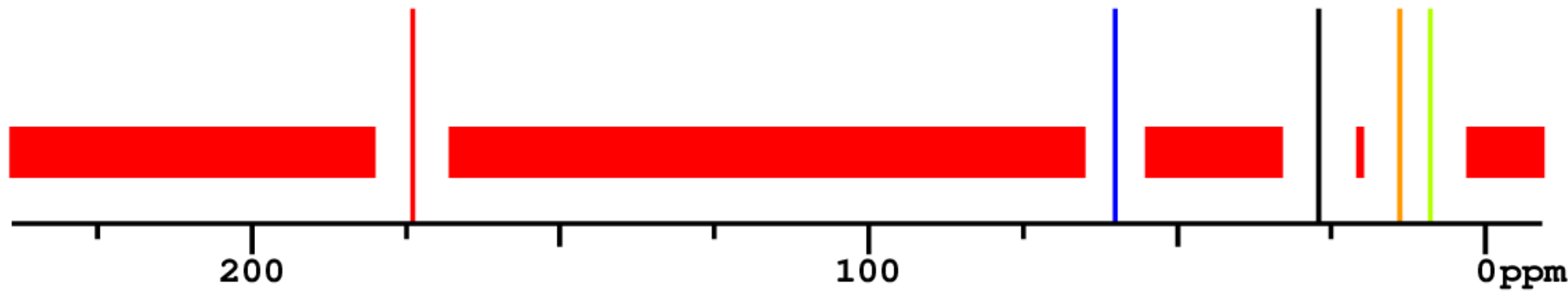
Structure Proposal #4

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>FKRCODPIKNEYAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



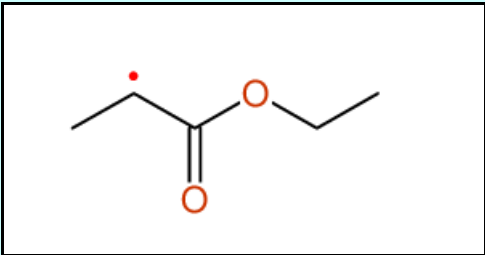
Experimental shift values

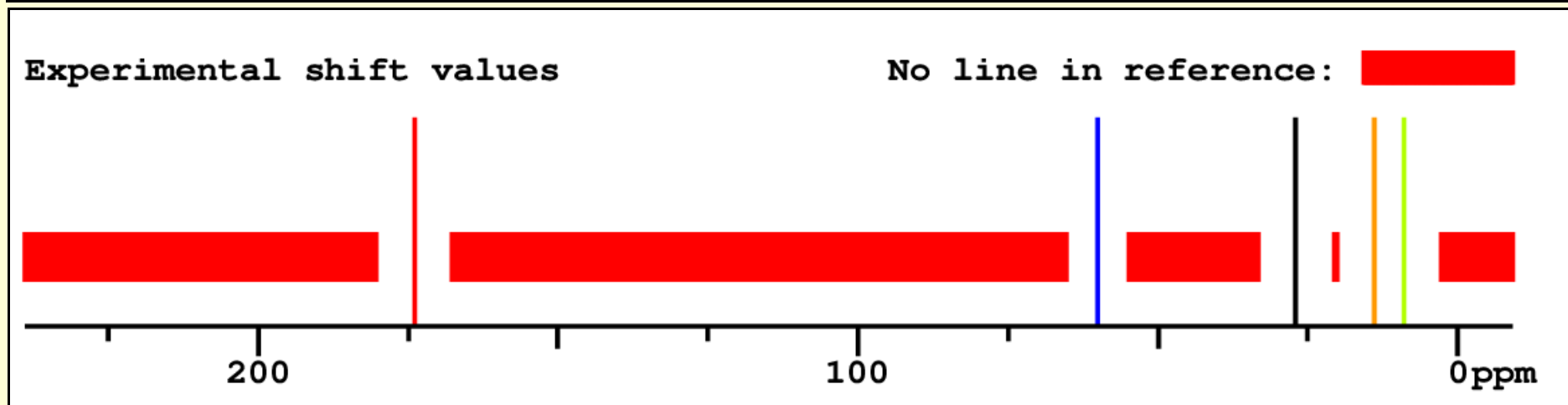
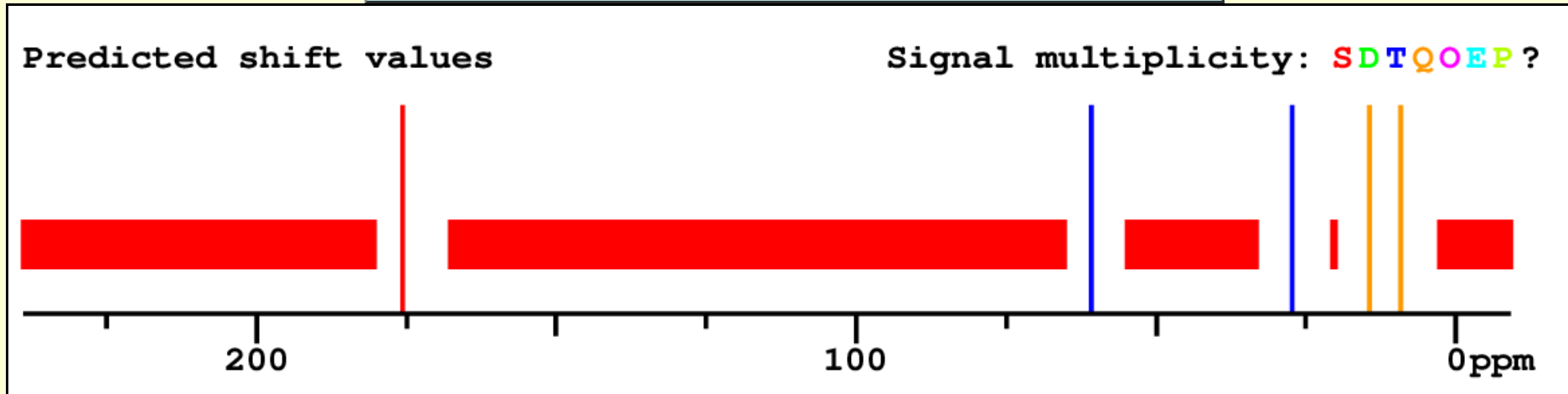
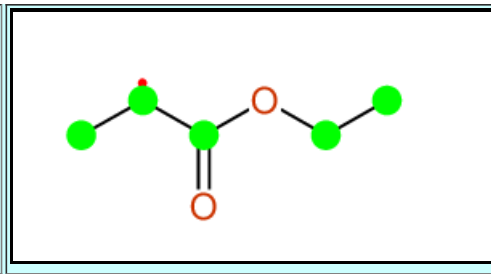
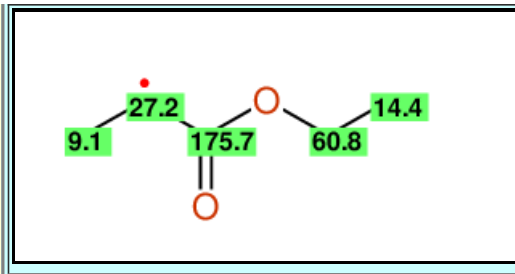
No line in reference: 



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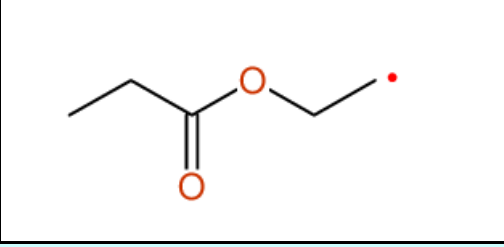
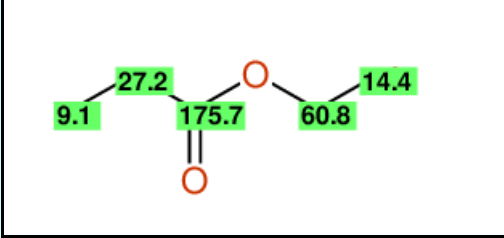
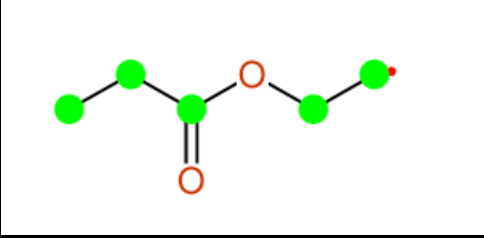
Structure Proposal #5

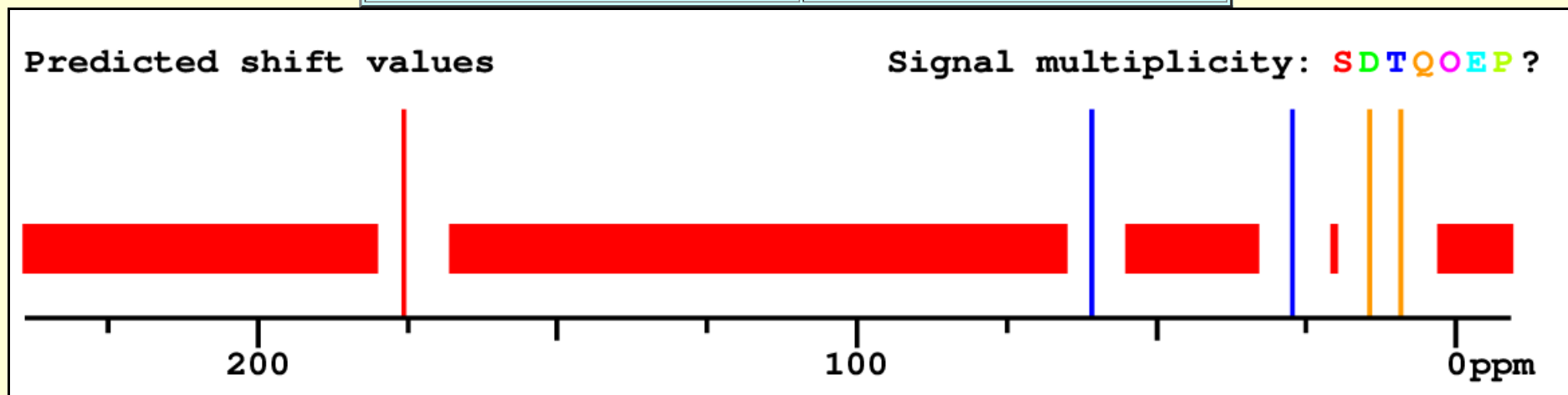
Structure	Similarity Measure
	<p>Deviation = 0.87 ppm</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 101.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>UPRLWNPAOPKPCE</p>
Predicted Chemical Shiftvalues	Matching Map



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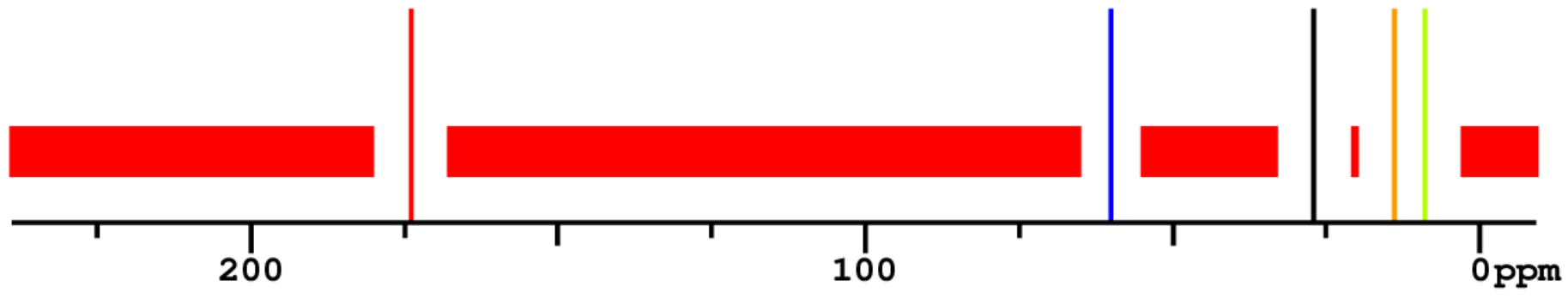
Structure Proposal #6

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
	



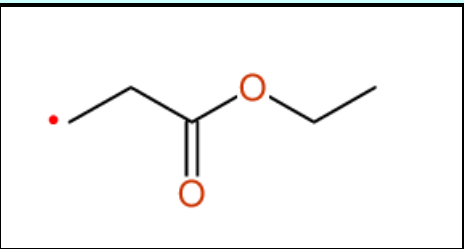
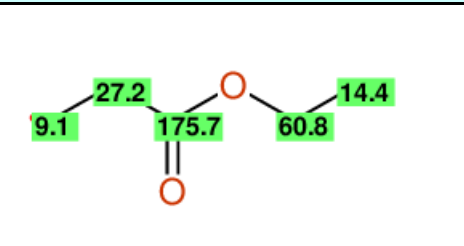
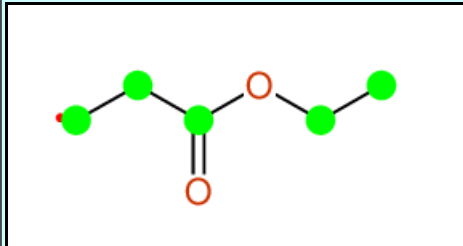
Experimental shift values

No line in reference: 



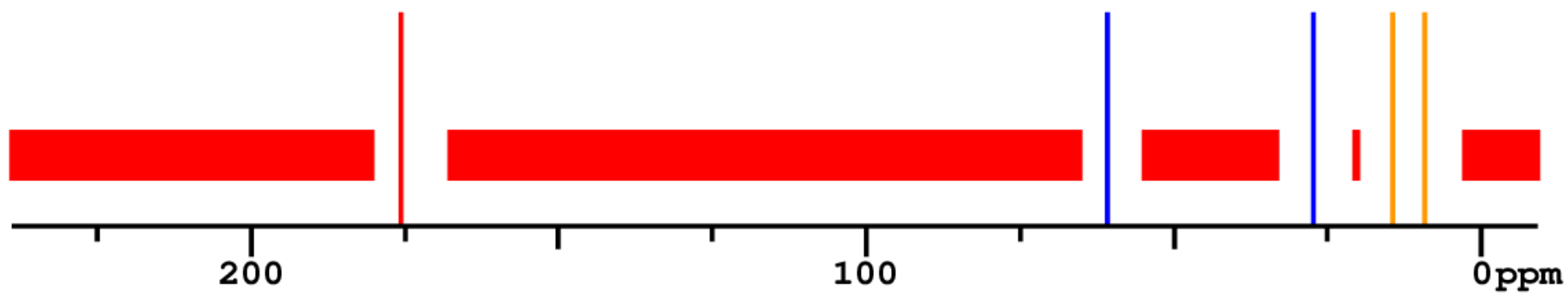
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Structure Proposal #7

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
	

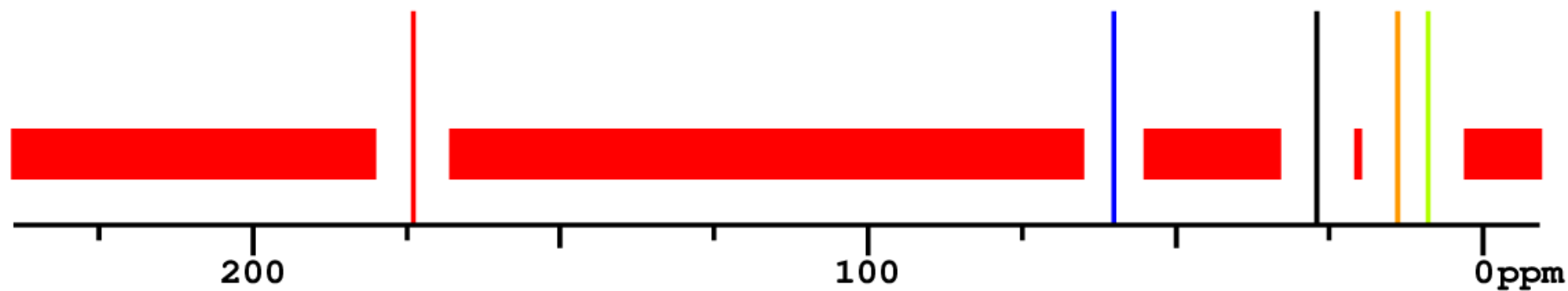
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

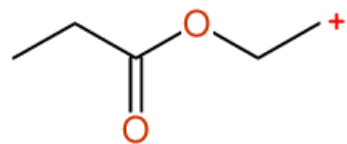
No line in reference: [red bar]



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Structure Proposal #8

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_9O_2^+$

MWT = 101.06

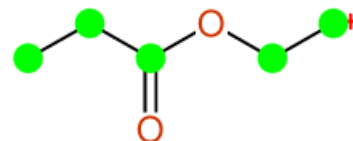
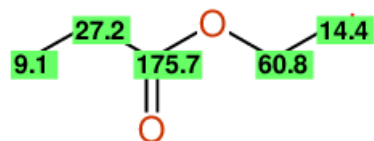
[PUBCHEM](#)

Search Web for this structure:

[GOKITYWXYBHPKU](#)

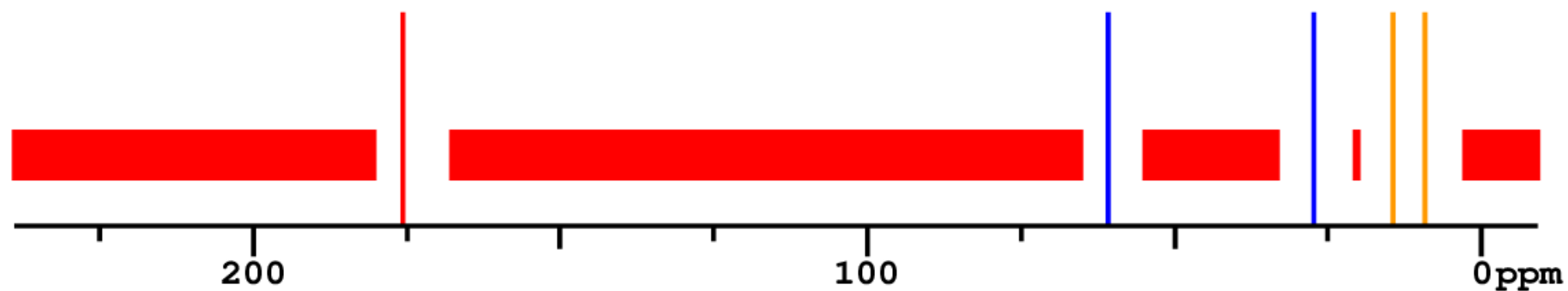
Predicted Chemical Shiftvalues

Matching Map



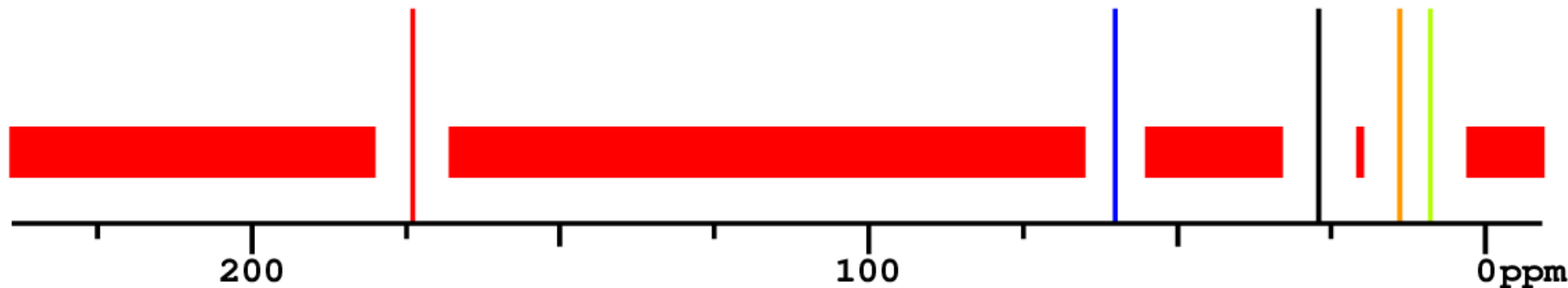
Predicted shift values

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



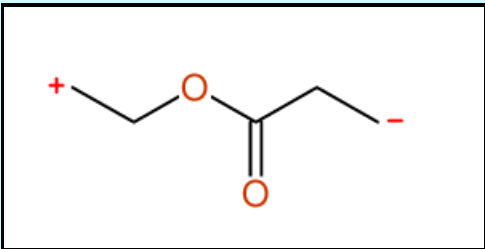
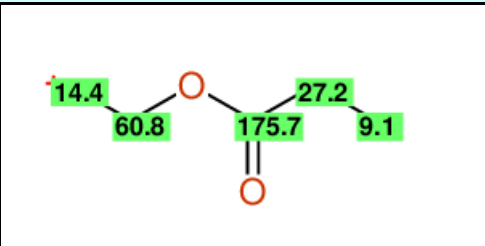
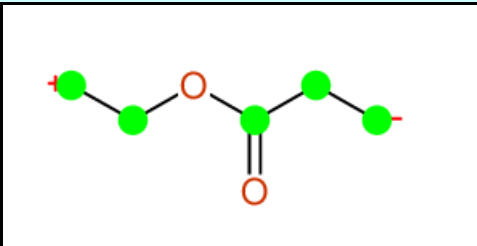
Experimental shift values

No line in reference: 



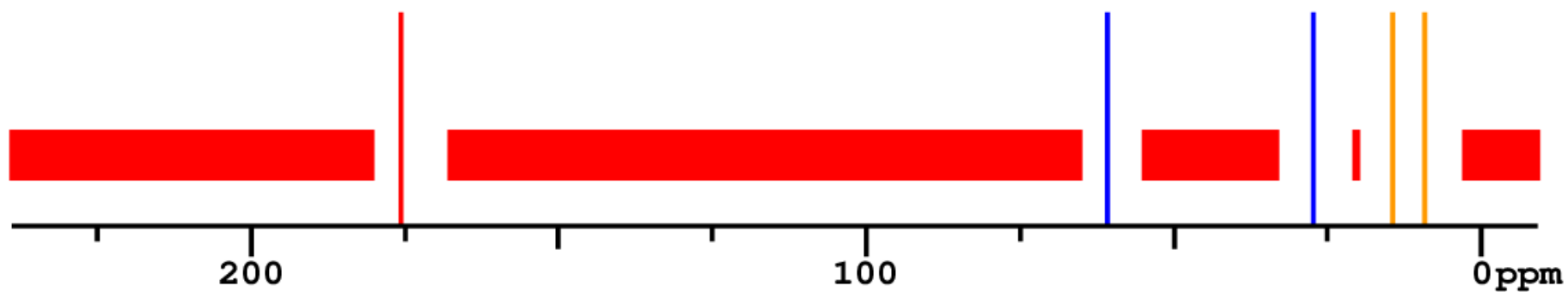
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Structure Proposal #9

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

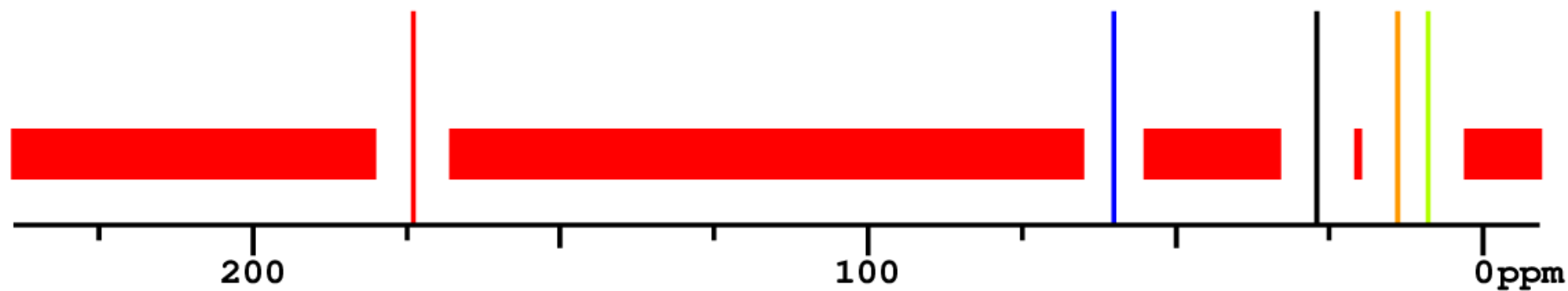
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

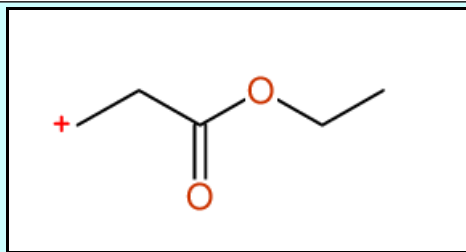
No line in reference: [red bar]



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Structure Proposal #10

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_9O_2^+$

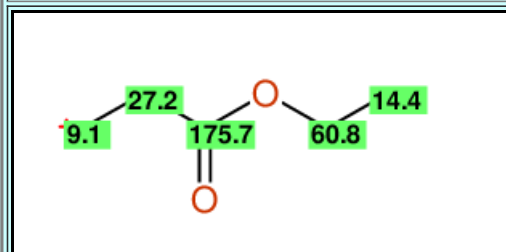
MWT = 101.06

[PUBCHEM](#)

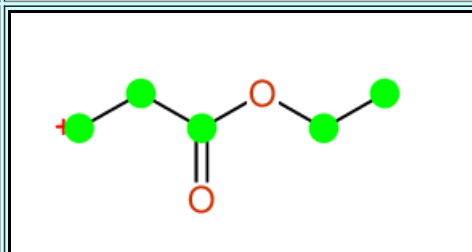
Search Web for this structure:

[MUQMZQYQIIZBIT](#)

Predicted Chemical Shiftvalues

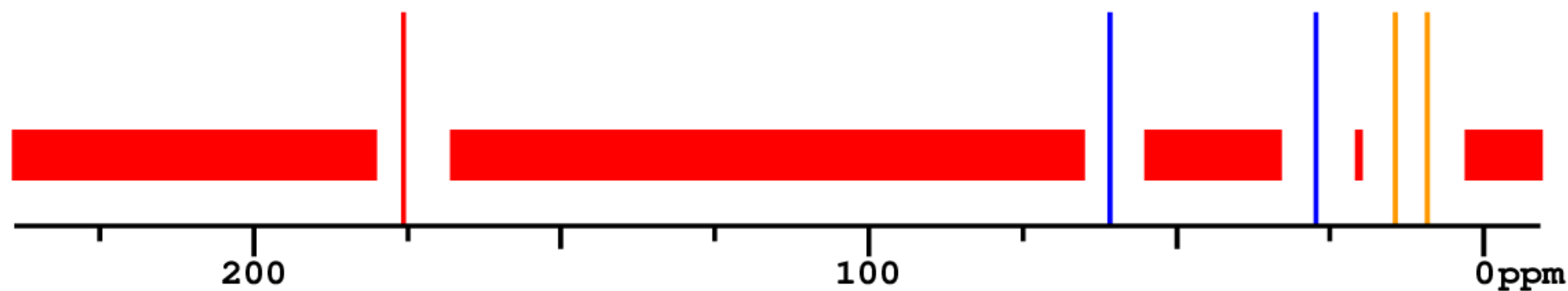


Matching Map




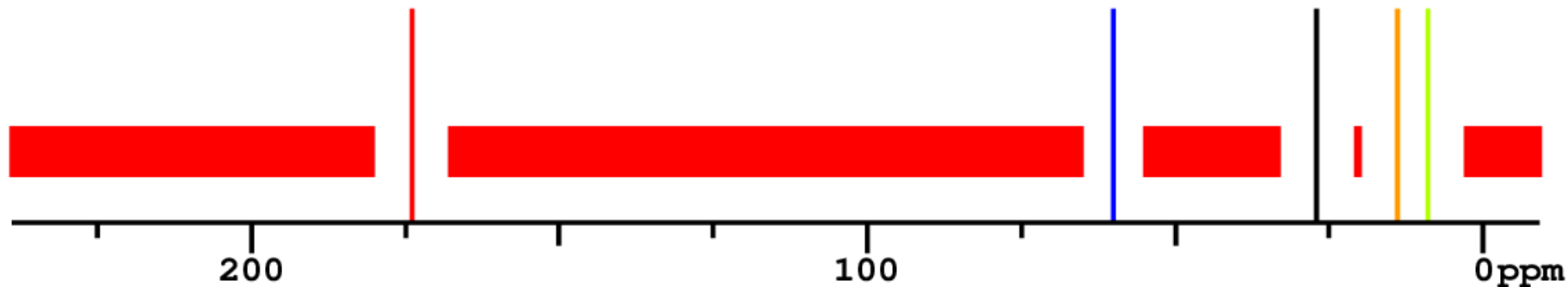
Predicted shift values

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



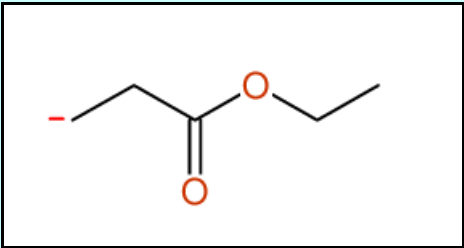
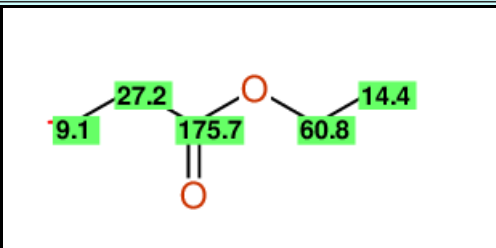
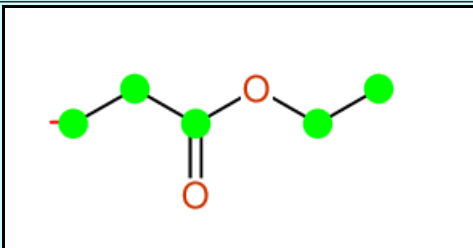
Experimental shift values

No line in reference: 



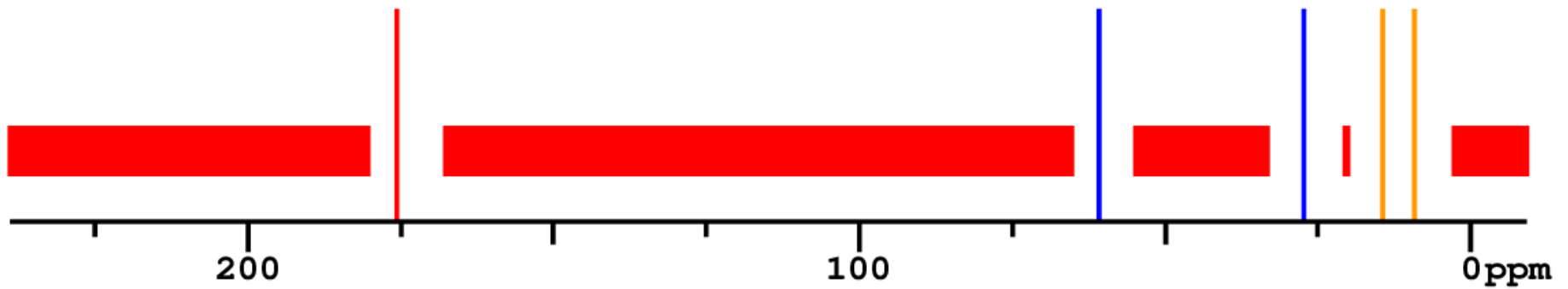
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Structure Proposal #11

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

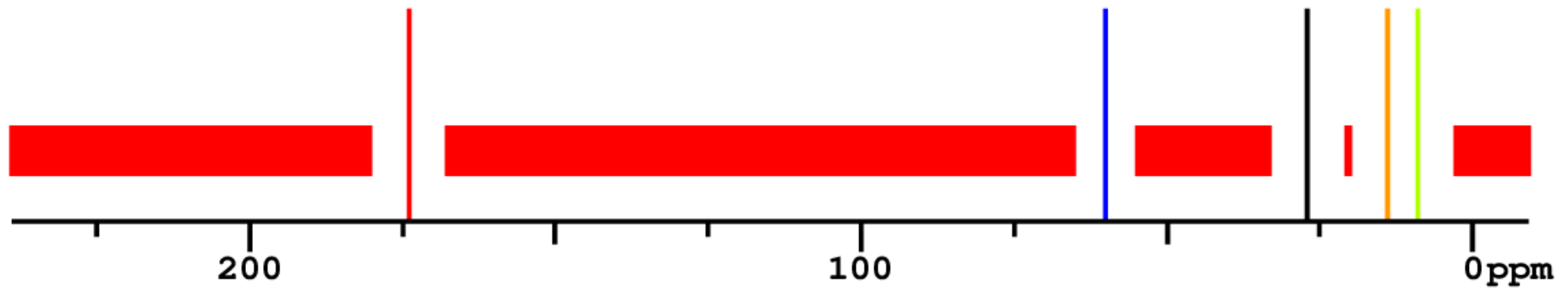
Predicted shift values

Signal multiplicity: S D T Q O E P ?



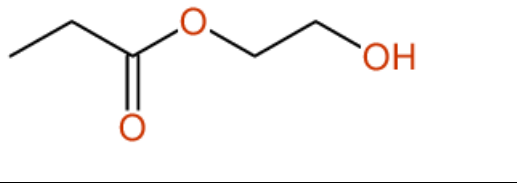
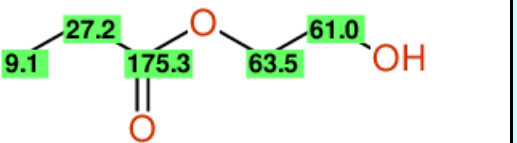
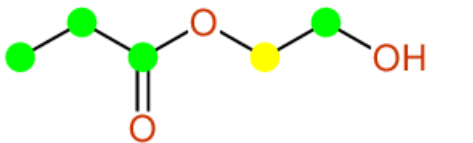
Experimental shift values

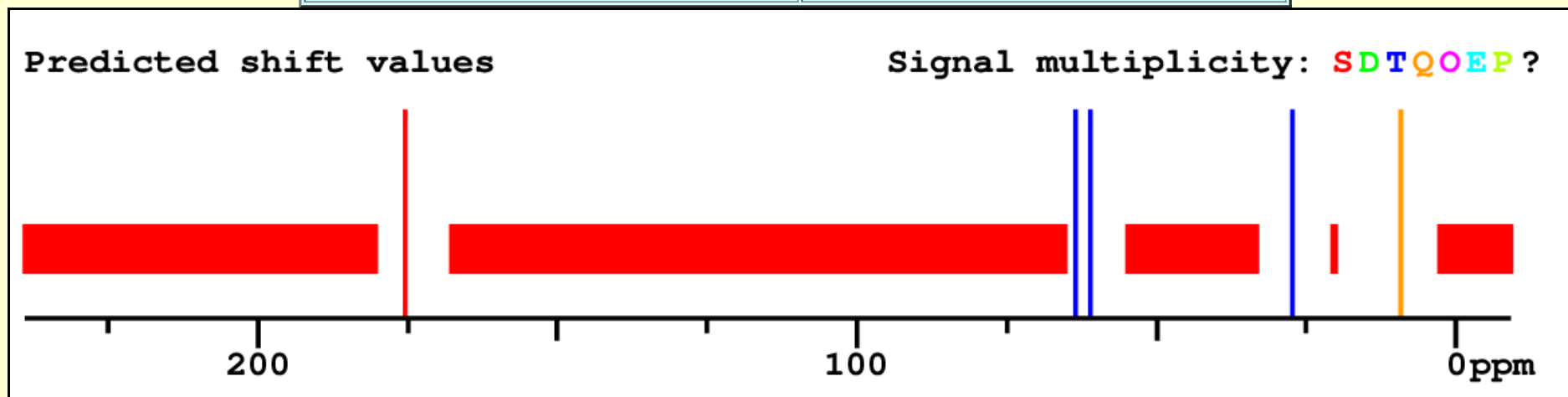
No line in reference: [red bar]



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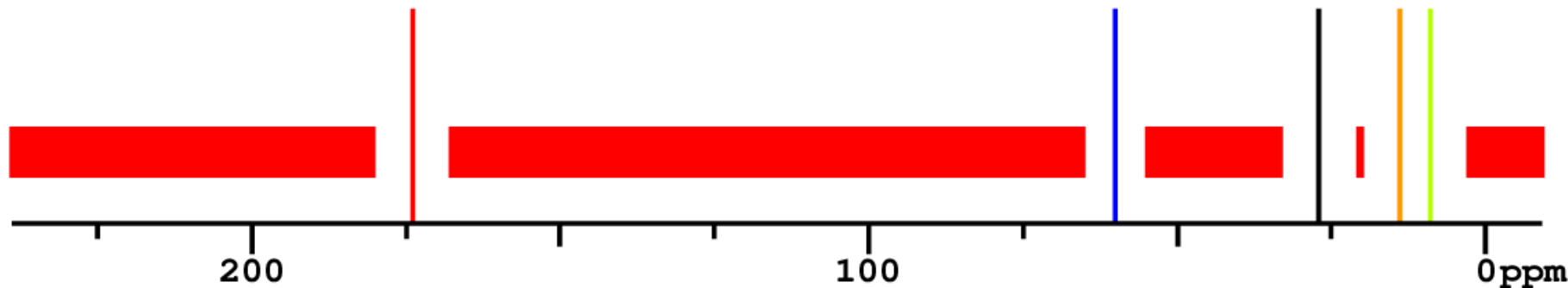
Structure Proposal #12

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



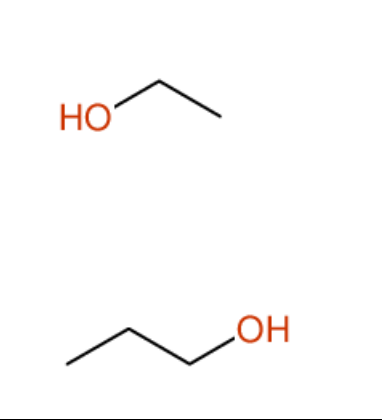
Experimental shift values

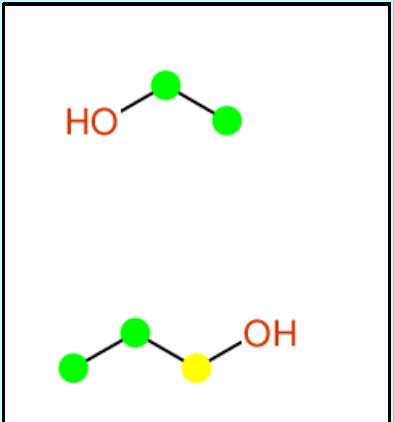
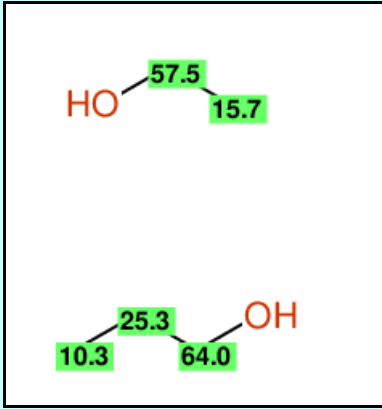
No line in reference: 



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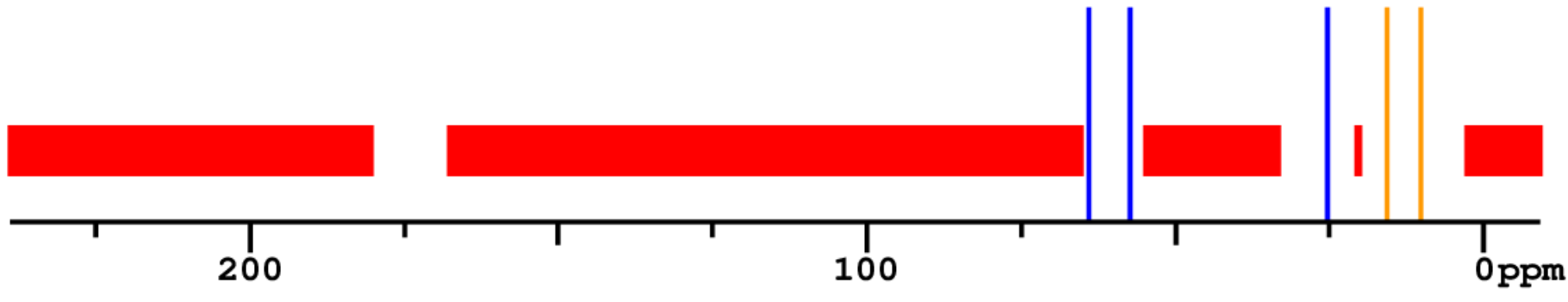
Structure Proposal #13

Structure	Similarity Measure
 <p>The image shows two chemical structures of 1-butanol. The top structure is a skeletal structure with the hydroxyl group (HO) explicitly labeled in red. The bottom structure is a skeletal structure with the hydroxyl group (OH) explicitly labeled in red.</p>	<p>Deviation = 2.62 ppm</p> <p>$C_5H_{14}O_2$</p> <p>MWT = 106.06</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>OMRDZQXXMYCHBU</p>
Predicted Chemical Shiftvalues	Matching Map



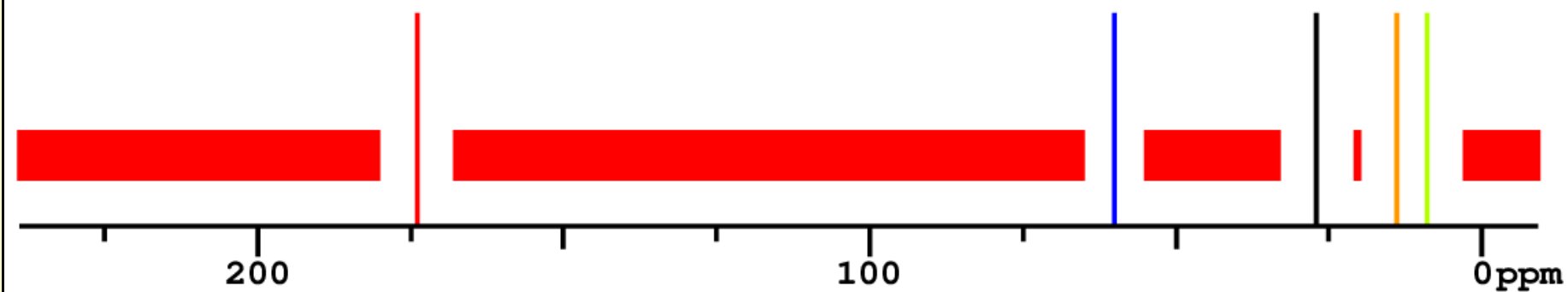
Predicted shift values

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



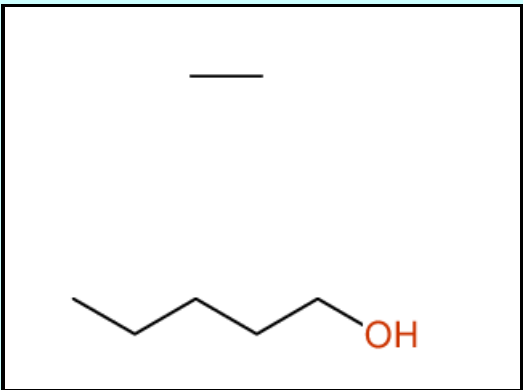
Experimental shift values

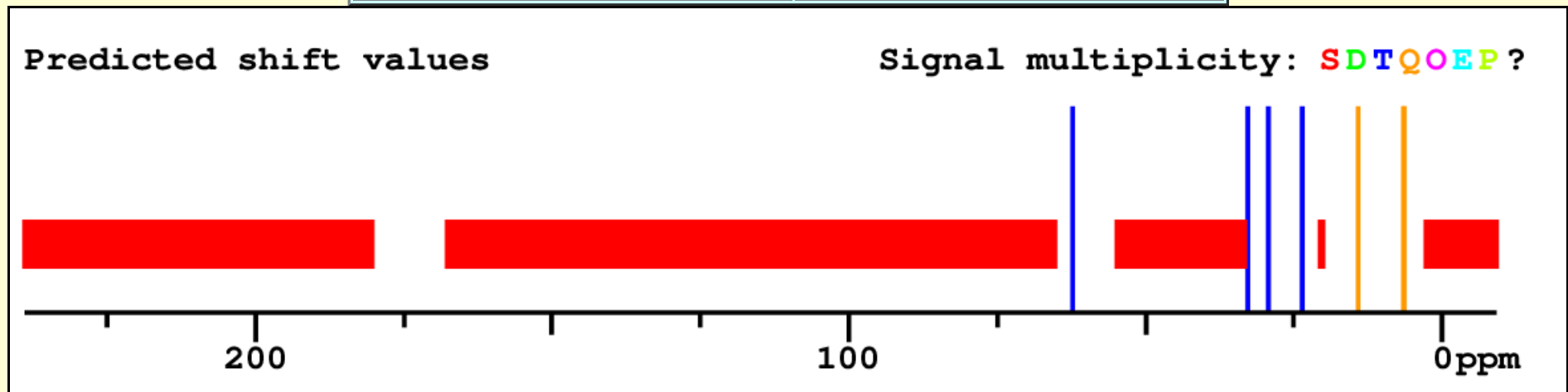
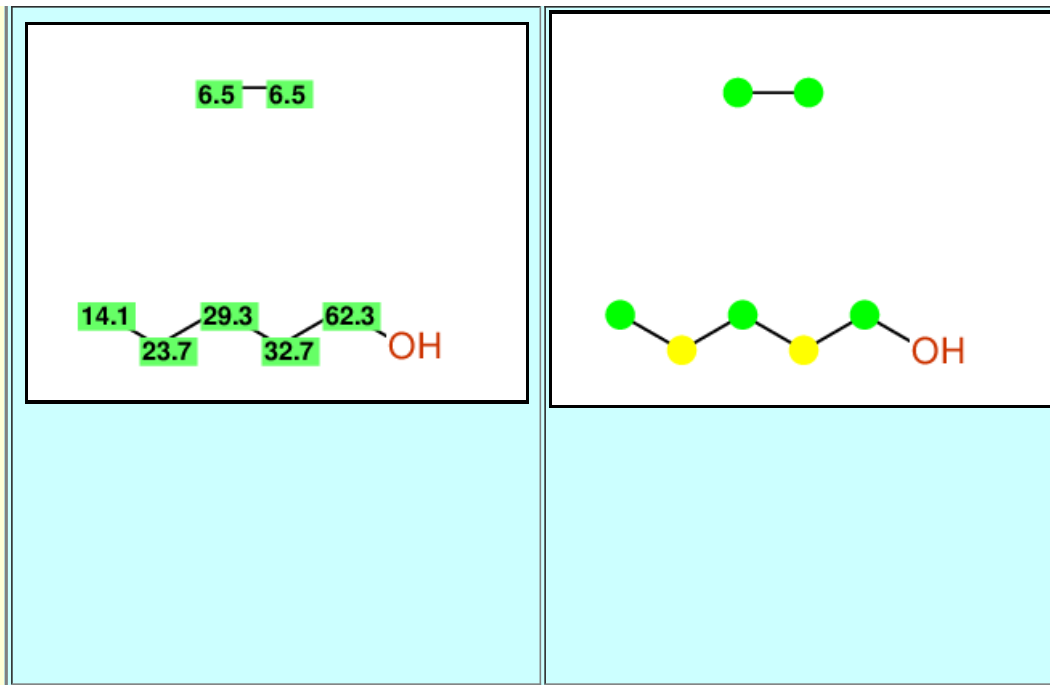
No line in reference: 



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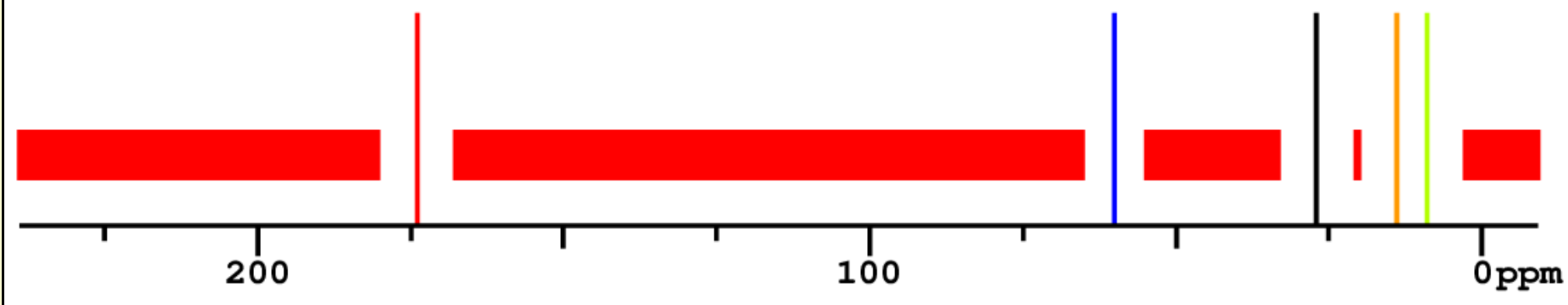
Structure Proposal #14

Structure	Similarity Measure
 <p>Chemical structure of 1-hexanol (SMILES: <chem>CCCCCCO</chem>) is shown in a box. The structure is a zigzag line representing a six-carbon chain with a hydroxyl group (-OH) attached to the first carbon.</p>	<p>Deviation = 2.98 ppm</p> <p>$C_7H_{18}O$</p> <p>MWT = 118.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>ZARMDFHSJSIZKQ</p>
Predicted Chemical Shiftvalues	Matching Map



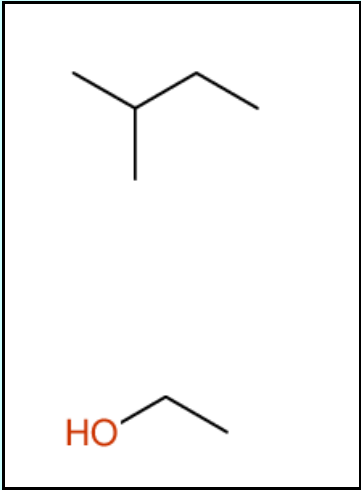
Experimental shift values

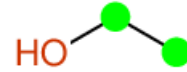
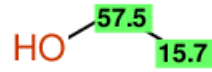
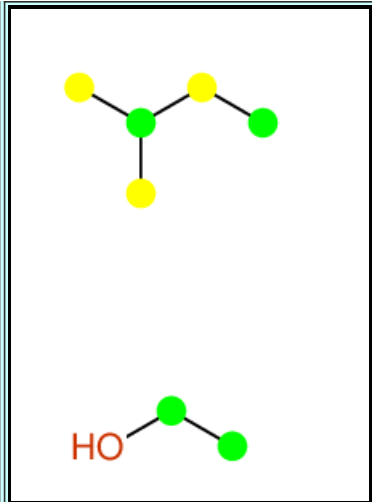
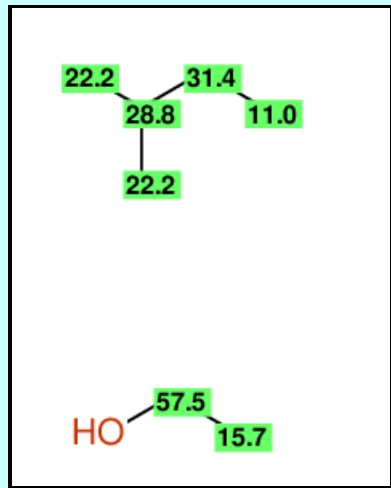
No line in reference: ████████



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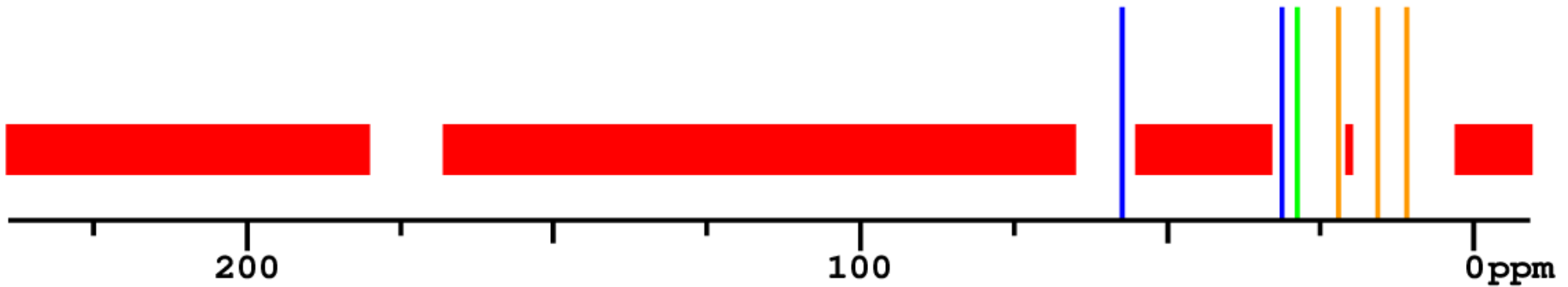
Structure Proposal #15

Structure	Similarity Measure
	<p>Deviation = 3.16 ppm</p> <p>$C_7H_{18}O$</p> <p>MWT = 118.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>FOXQTCHXXJKLNK</p>
Predicted Chemical Shiftvalues	Matching Map



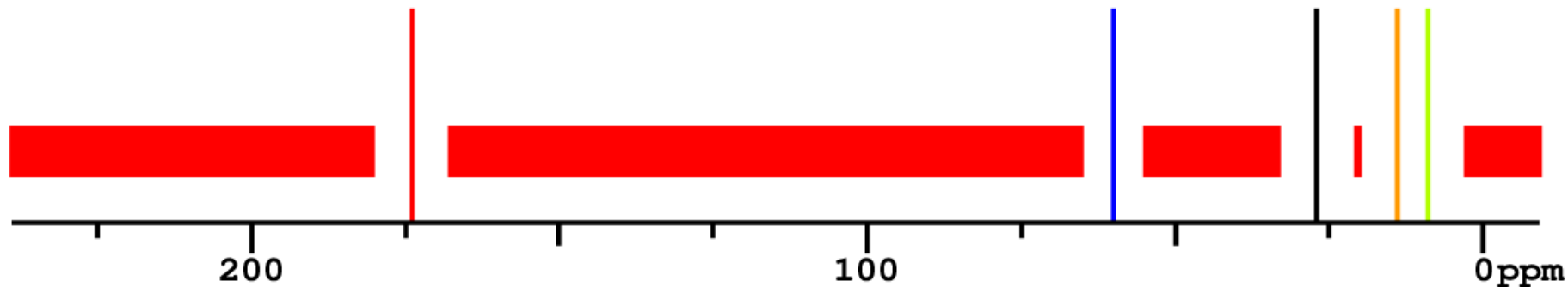
Predicted shift values

Signal multiplicity: S D T Q O E P ?



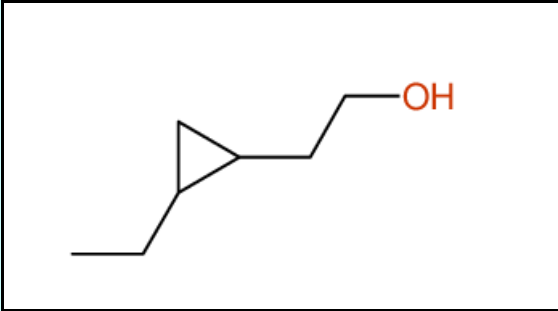
Experimental shift values

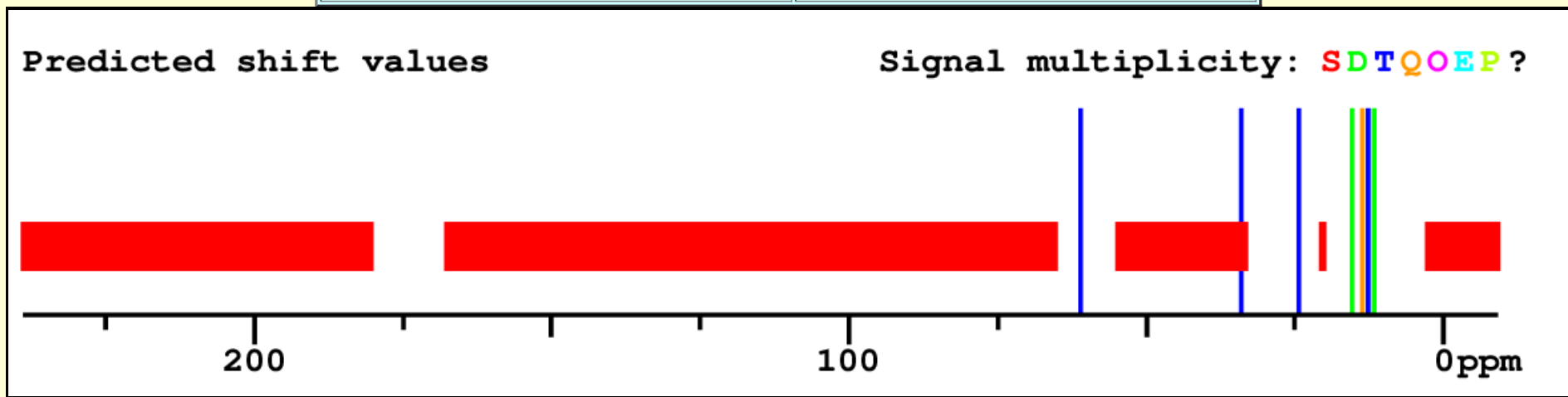
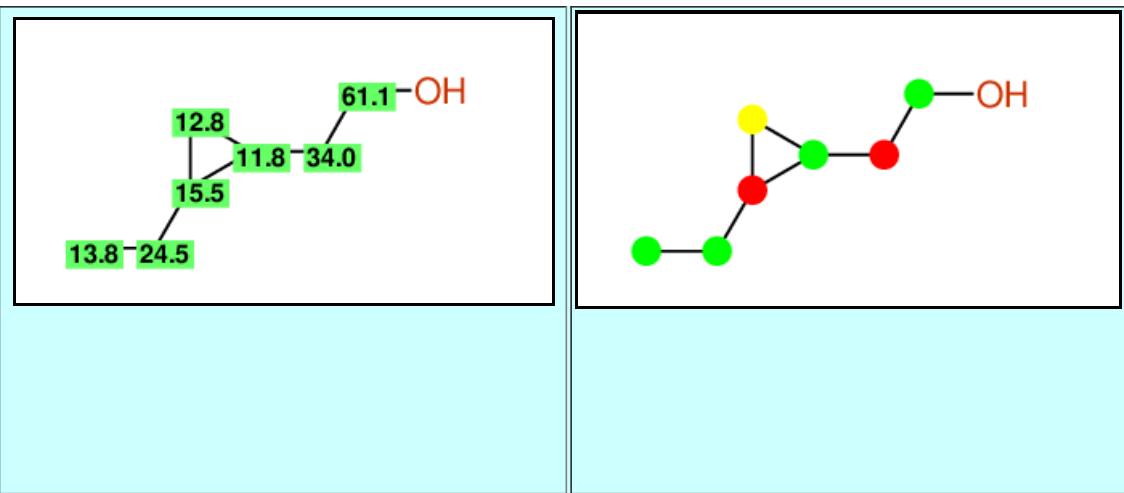
No line in reference: 



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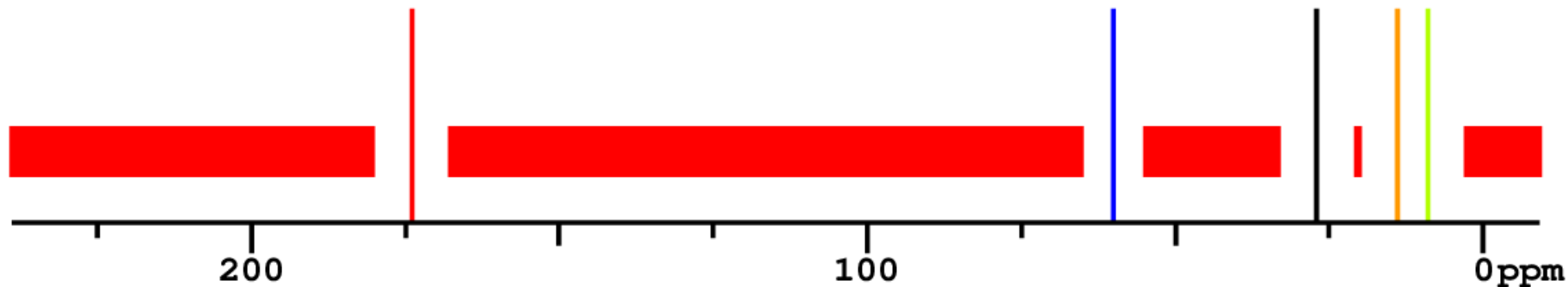
Structure Proposal #16

Structure	Similarity Measure
	<p>Deviation = 3.49 ppm (Different pattern)</p> <p>$C_7H_{14}O$</p> <p>MWT = 114.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>IPKMDCPNAOYUEB</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



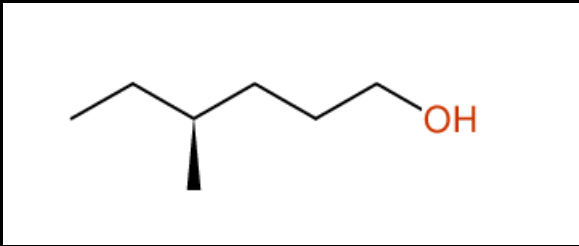
Experimental shift values

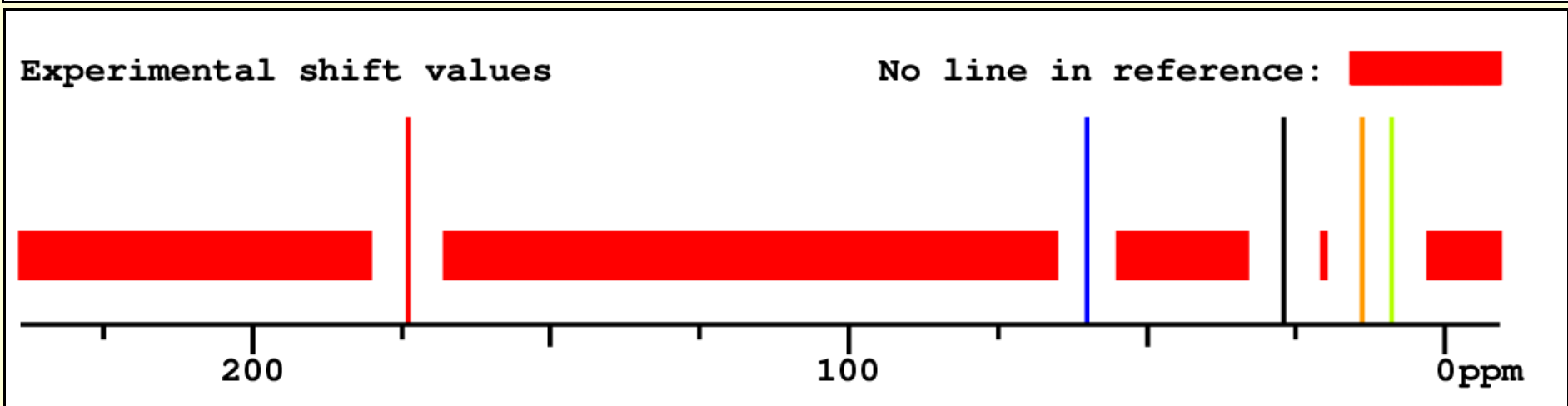
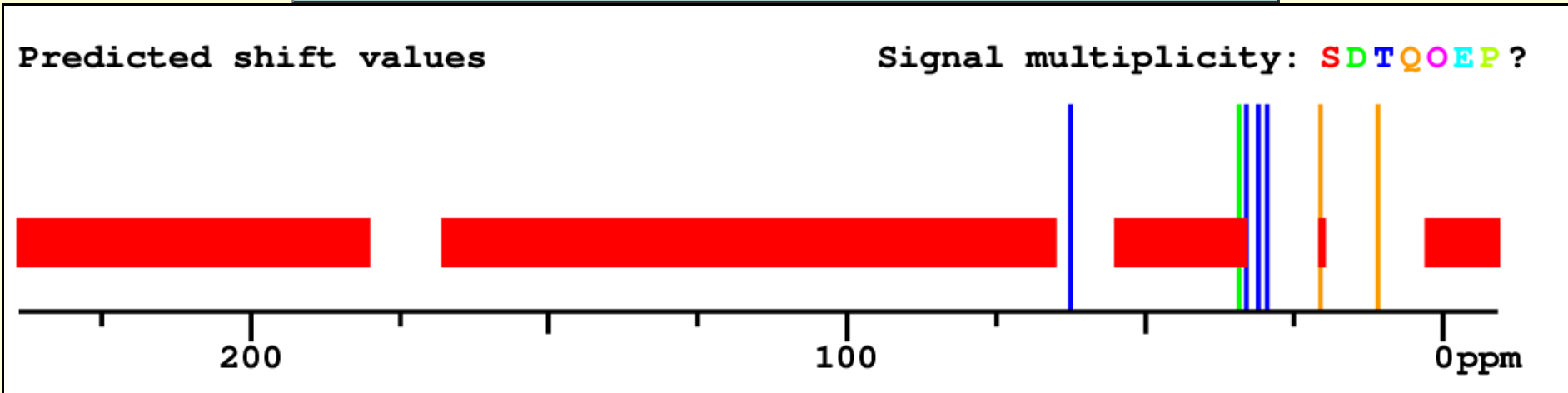
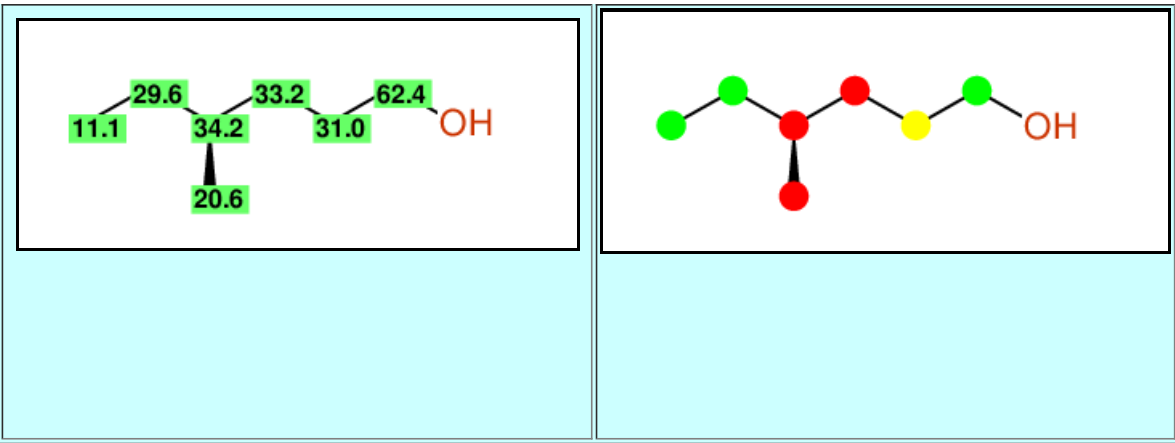
No line in reference: 



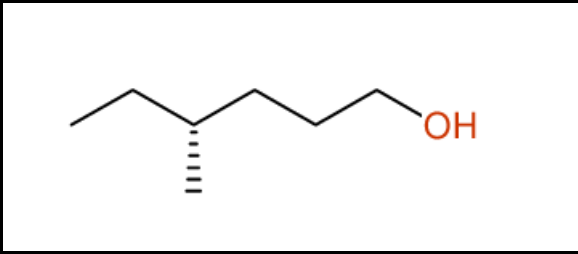
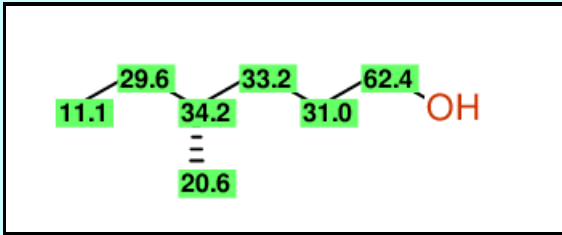
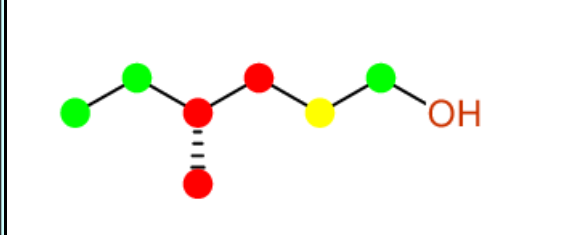
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Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 4.01 ppm (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>YNPVNLWKVZZBTM</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map

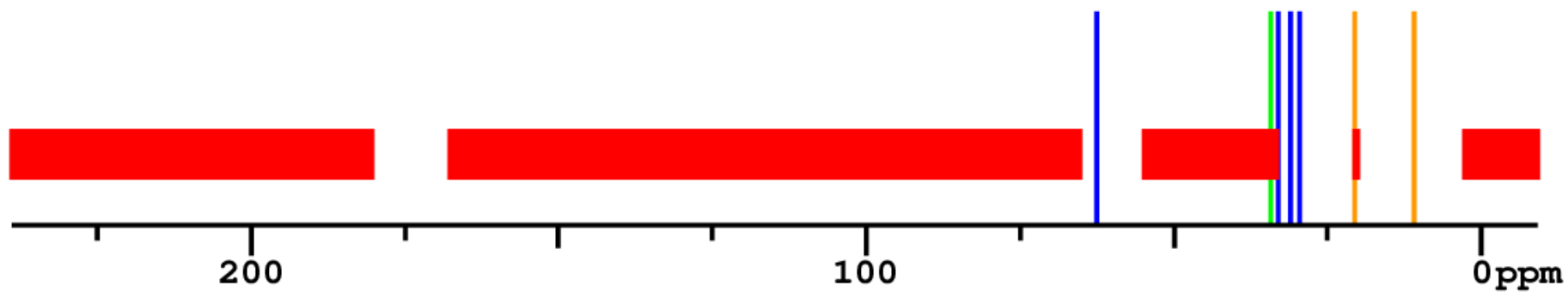


Structure Proposal #18

Structure	Similarity Measure
	<p>Deviation = 4.01 ppm (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>YNPVNLWKVZZBTM</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map
	

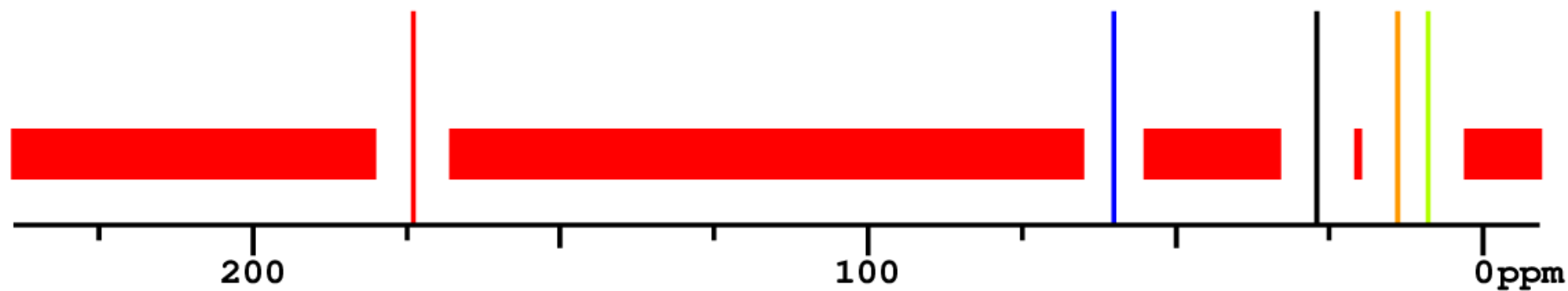
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

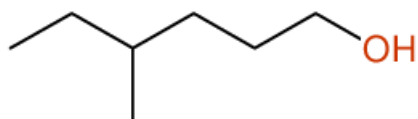
No line in reference: [red bar]



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Structure Proposal #19

Structure	Similarity Measure



Deviation = 4.01 ppm
(Different pattern)

$C_7H_{16}O$

MWT = 116.08

[PUBCHEM](#)

Search Web for this structure:

[YNPVNLWKVZZBTM](#)

[Availability](#)

Predicted Chemical Shiftvalues

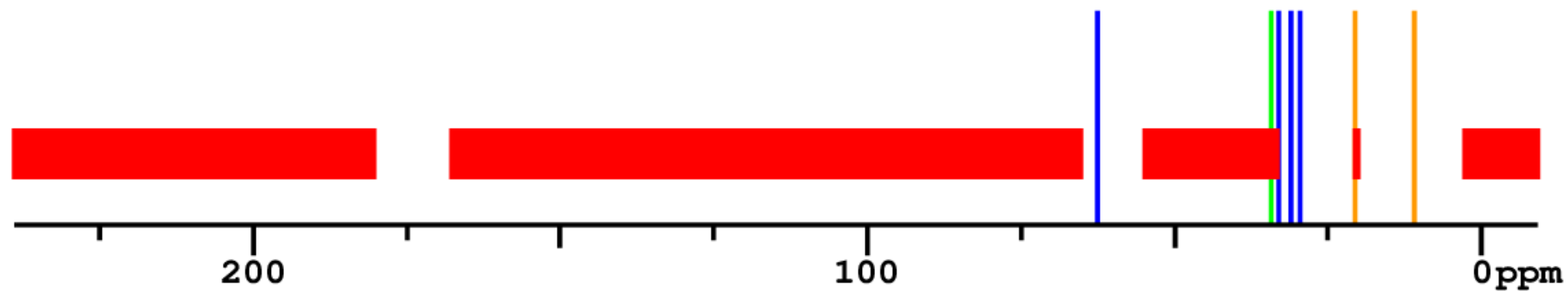


Matching Map



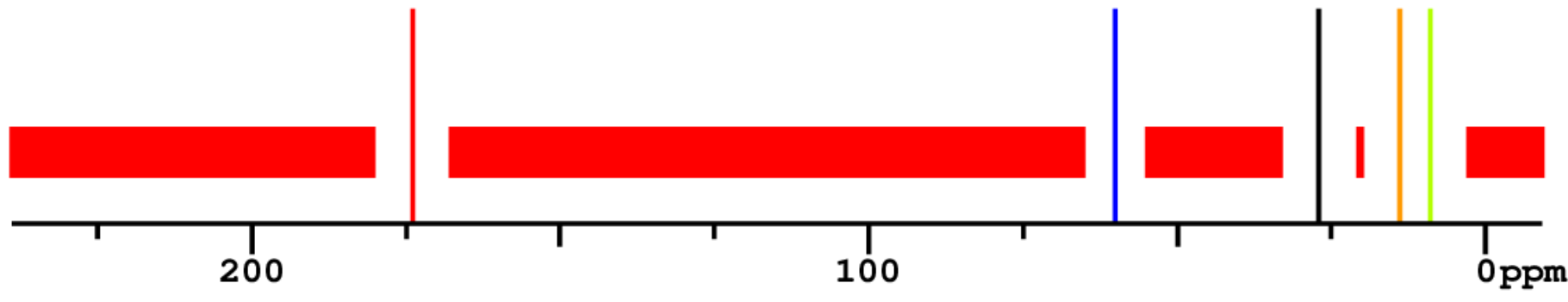
Predicted shift values

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



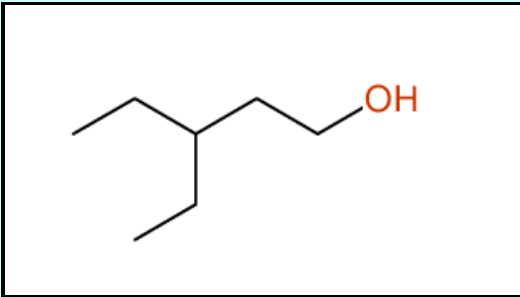
Experimental shift values

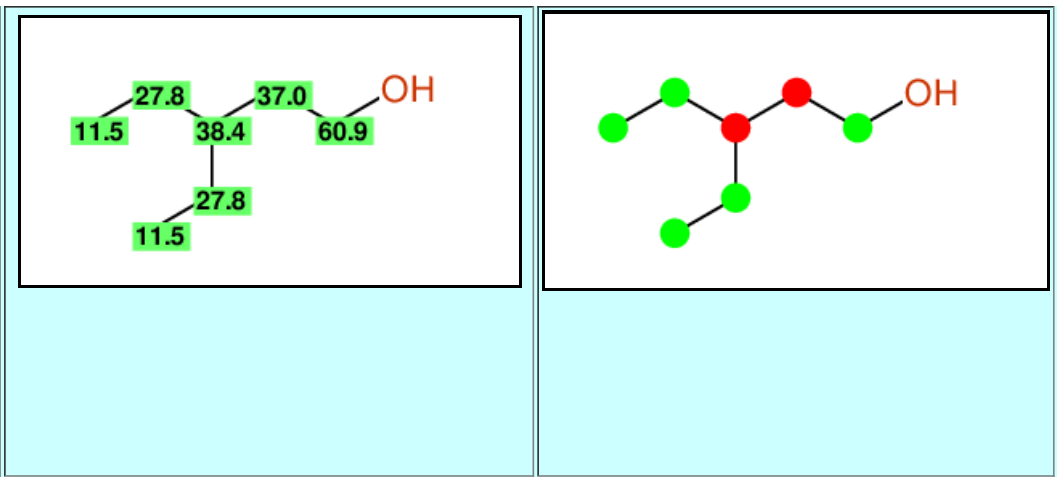
No line in reference: 



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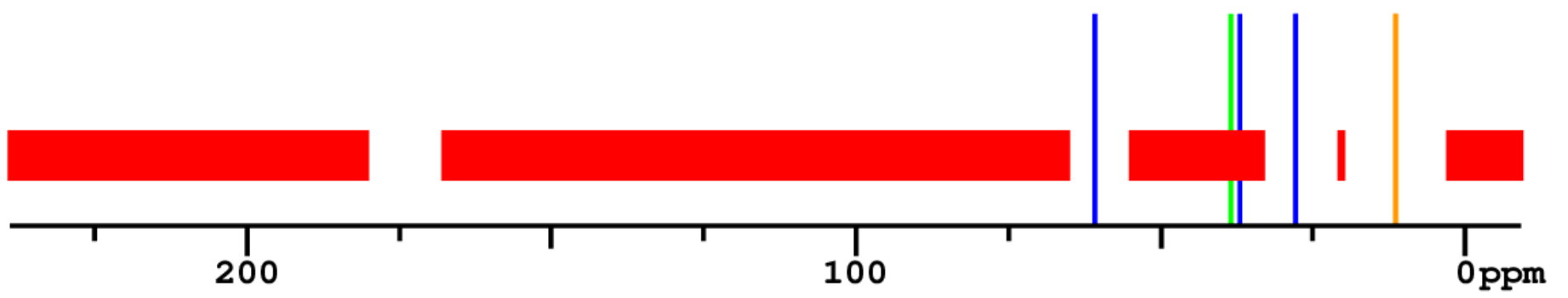
Structure Proposal #20

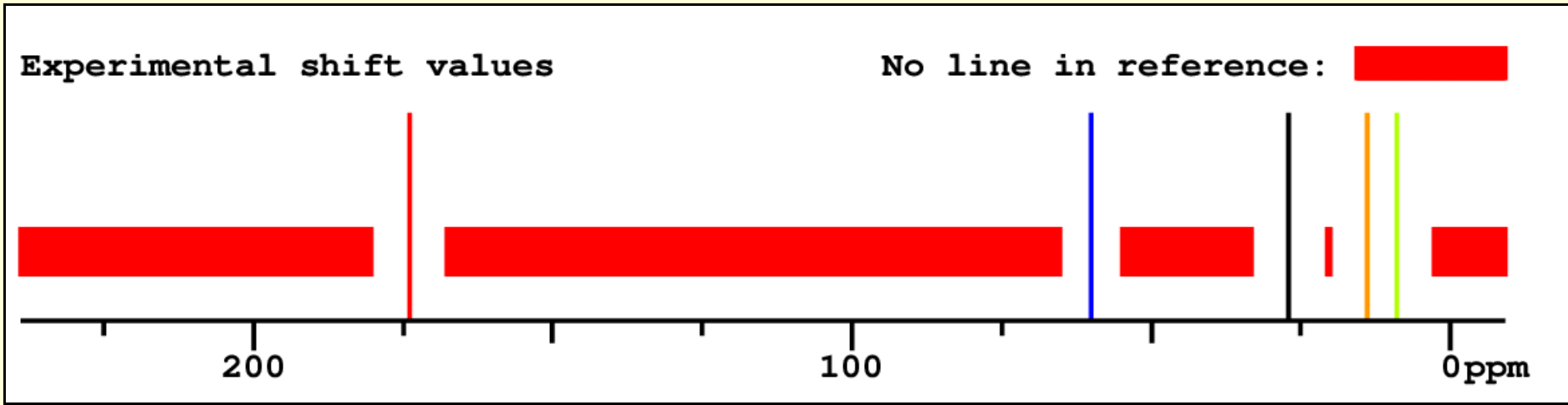
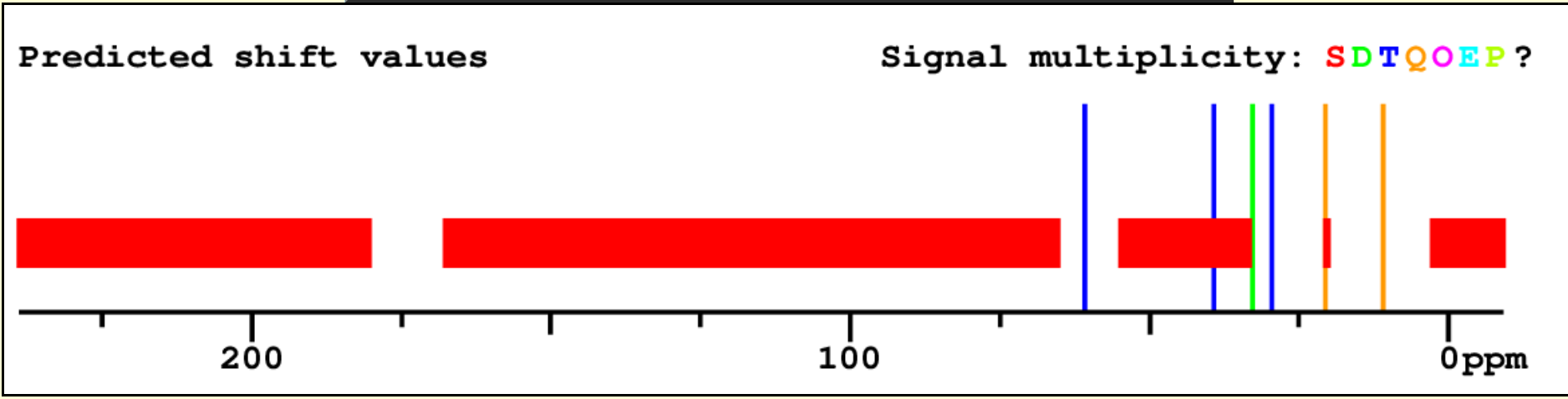
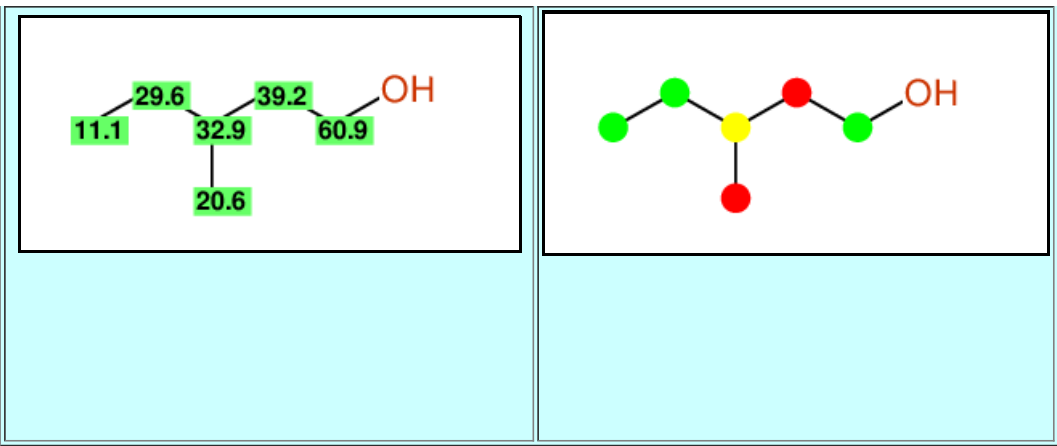
Structure	Similarity Measure
	<p>Deviation = 4.36 ppm (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>DVEFUHVWJONKR</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



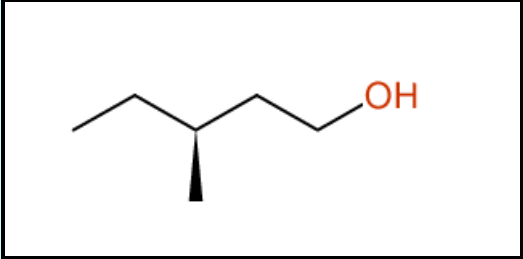
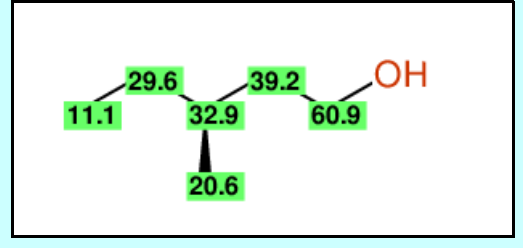
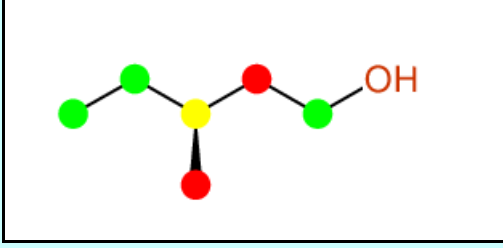
Predicted shift values

Signal multiplicity: S D T Q O E P ?



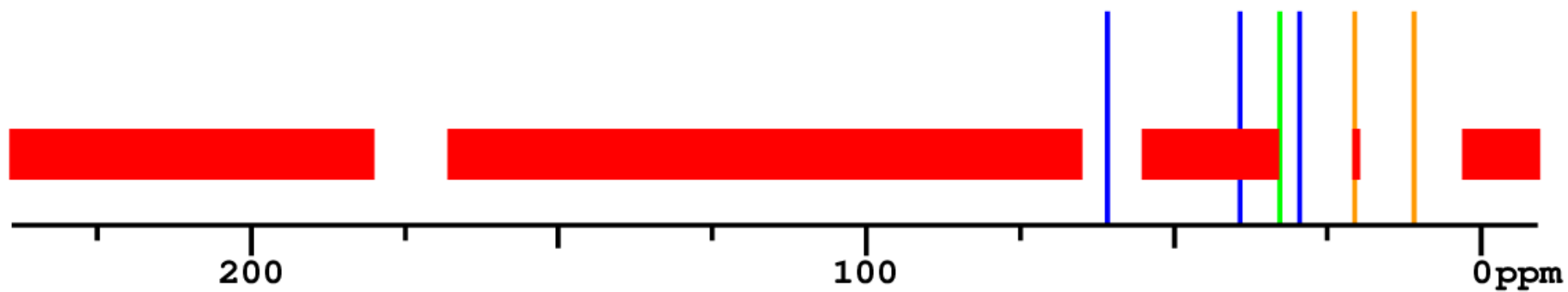


Structure Proposal #22

Structure	Similarity Measure
 <p>Chemical structure of 2-methyl-1-hexanol, showing a six-carbon chain with a methyl group on the second carbon and a hydroxyl group on the first carbon.</p>	<p>Deviation = 4.64 ppm (Different pattern)</p> <p>$C_6H_{14}O$</p> <p>MWT = 102.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>IWTBVKIGCDZRPL</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map
 <p>Chemical structure of 2-methyl-1-hexanol with predicted chemical shift values (ppm) for each carbon atom: 11.1, 29.6, 32.9, 39.2, and 60.9. The methyl group is labeled with 20.6 ppm.</p>	 <p>Matching map showing the correspondence between the chemical structure and the predicted shift values. The structure is color-coded: green for carbons 1, 2, and 5; red for carbons 3 and 6; and yellow for carbon 4. The methyl group is shown in red.</p>

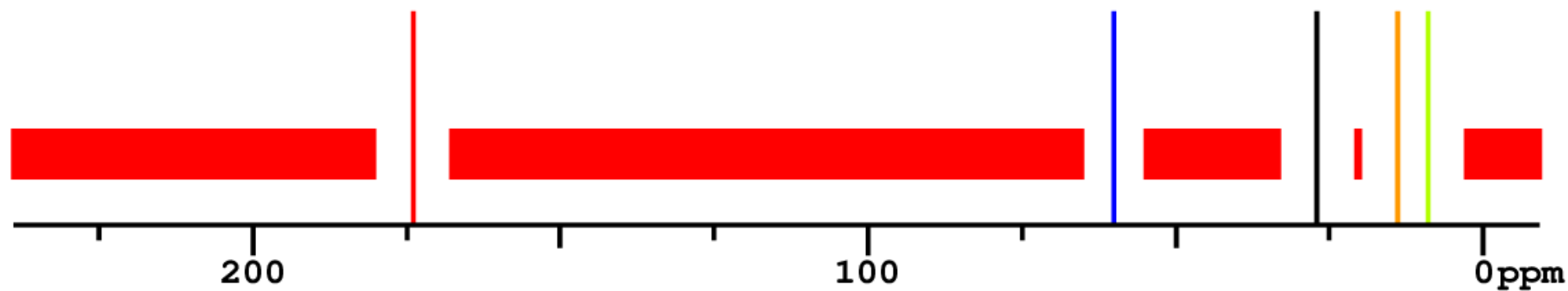
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

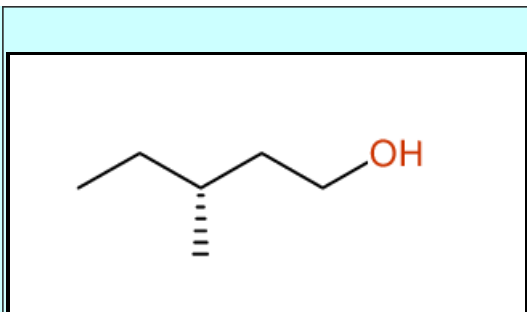
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Structure Proposal #23

Structure	Similarity Measure



Deviation = 4.64 ppm
(Different pattern)

$C_6H_{14}O$

MWT = 102.07

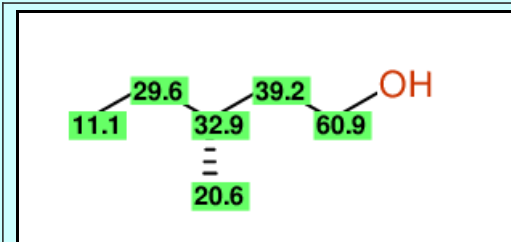
[PUBCHEM](#)

Search Web for this structure:

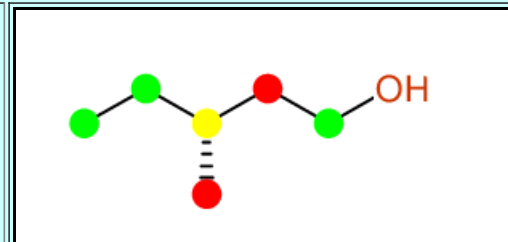
[IWTBVKIGCDZRPL](#)

[Availability](#)

Predicted Chemical Shiftvalues

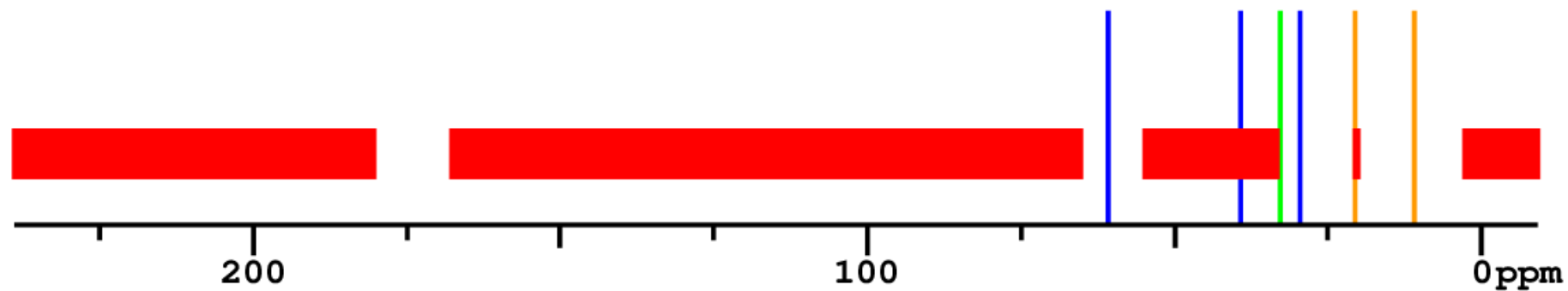


Matching Map



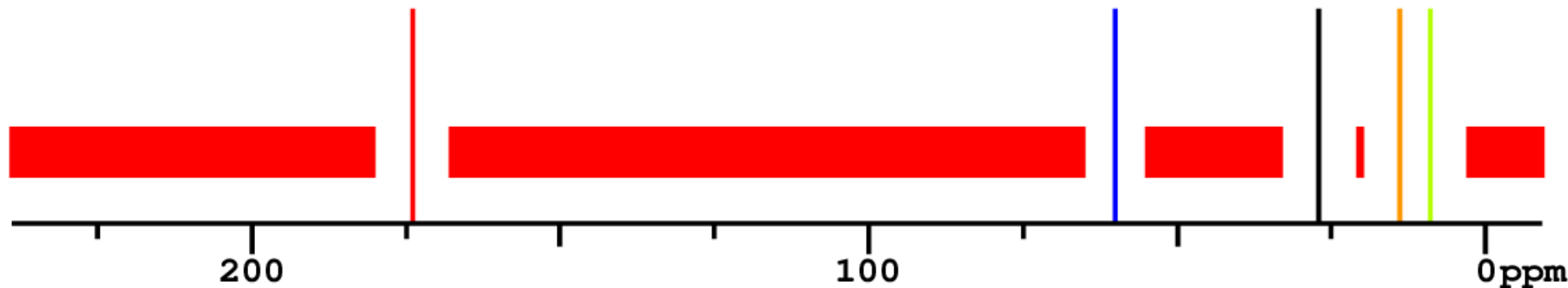
Predicted shift values

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



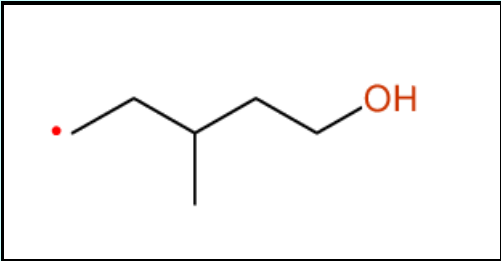
Experimental shift values

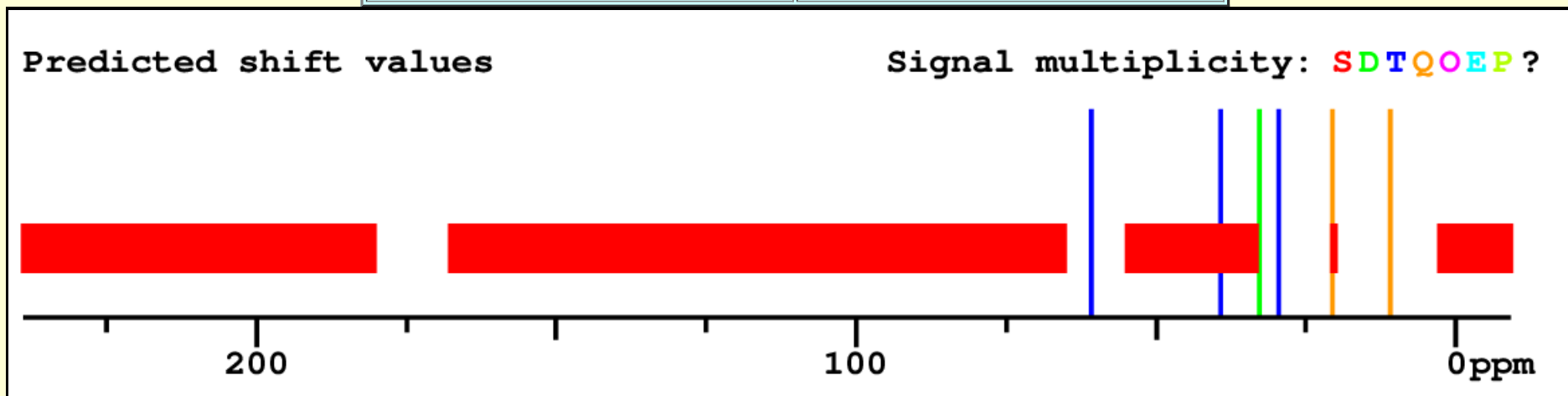
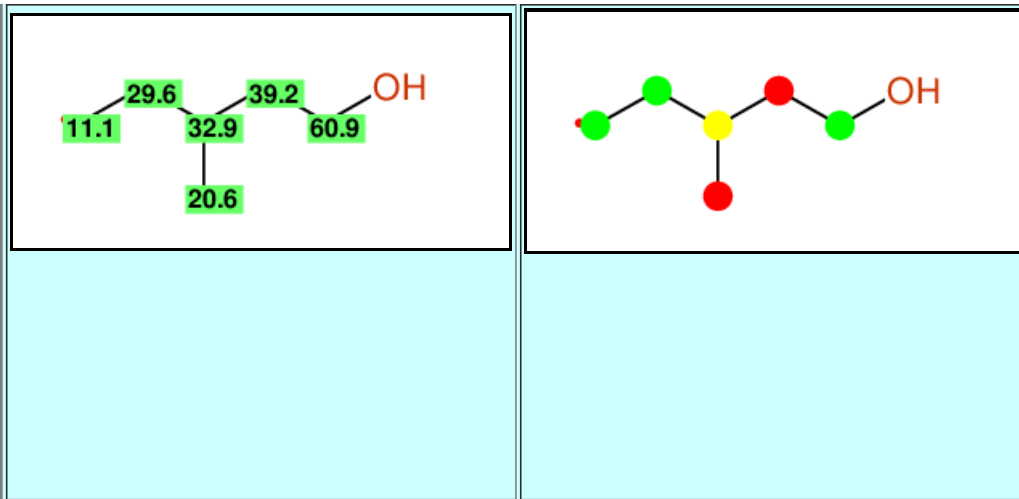
No line in reference: 



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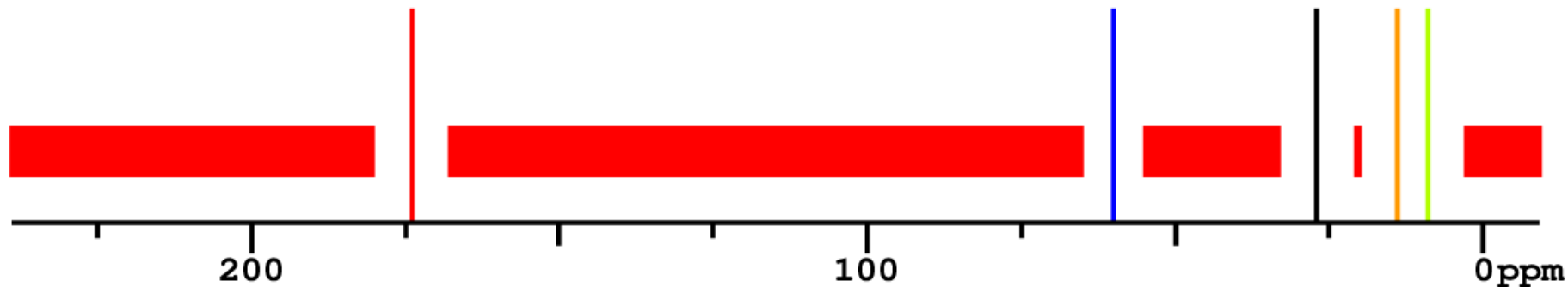
Structure Proposal #24

Structure	Similarity Measure
	<p>Deviation = 4.64 ppm (Different pattern)</p> <p>$C_6H_{13}O$</p> <p>MWT = 101.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>FCACGIMTGMLTKJ</p>
Predicted Chemical Shiftvalues	Matching Map



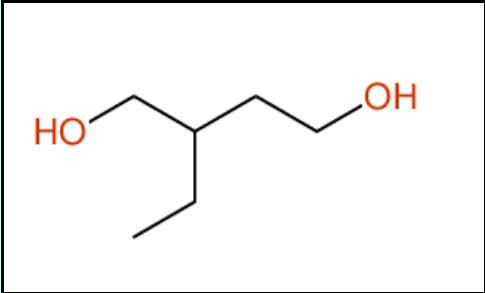
Experimental shift values

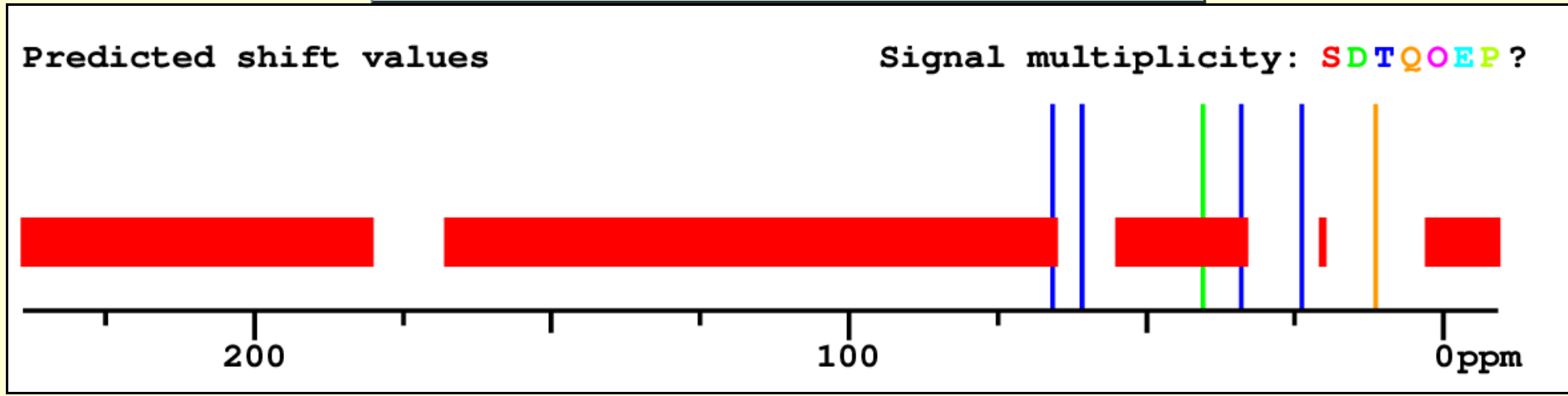
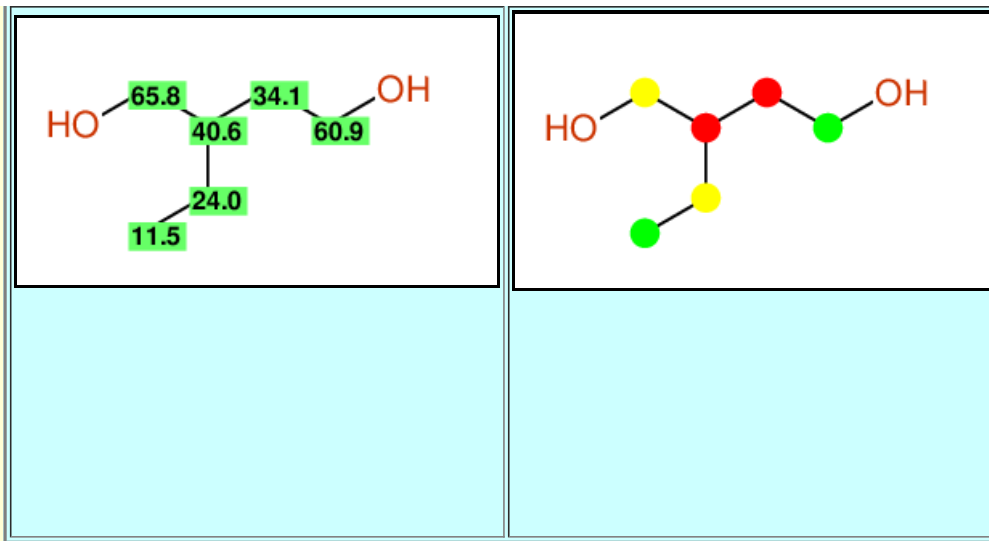
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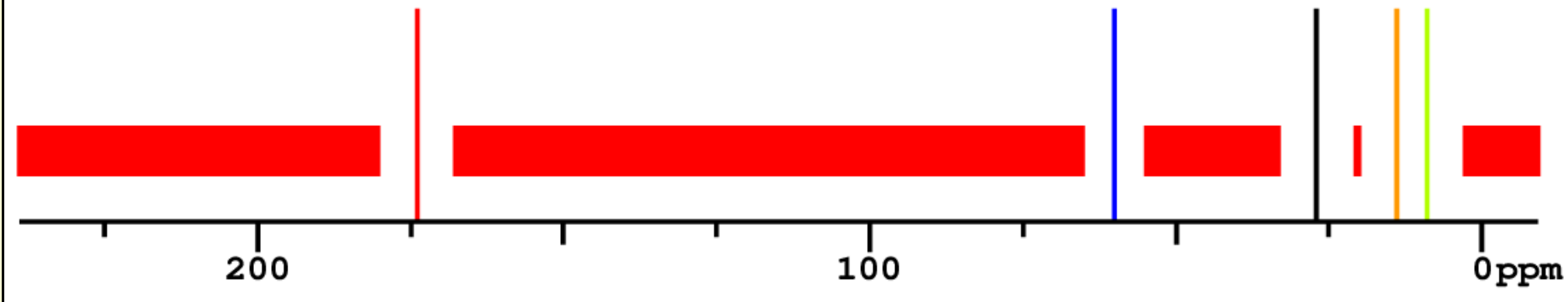
Structure Proposal #25

Structure	Similarity Measure
 <p>Chemical structure of 2-ethyl-1,5-hexanediol: <chem>CCCC(O)C(O)CC</chem></p>	<p>Deviation = 4.98 ppm (Different pattern)</p> <p>$C_6H_{14}O_2$</p> <p>MWT = 118.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>CYVMBANVYOZFIG</p>
Predicted Chemical Shiftvalues	Matching Map



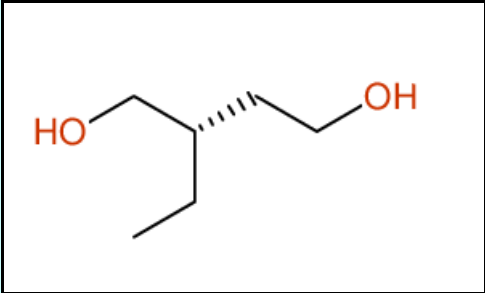
Experimental shift values

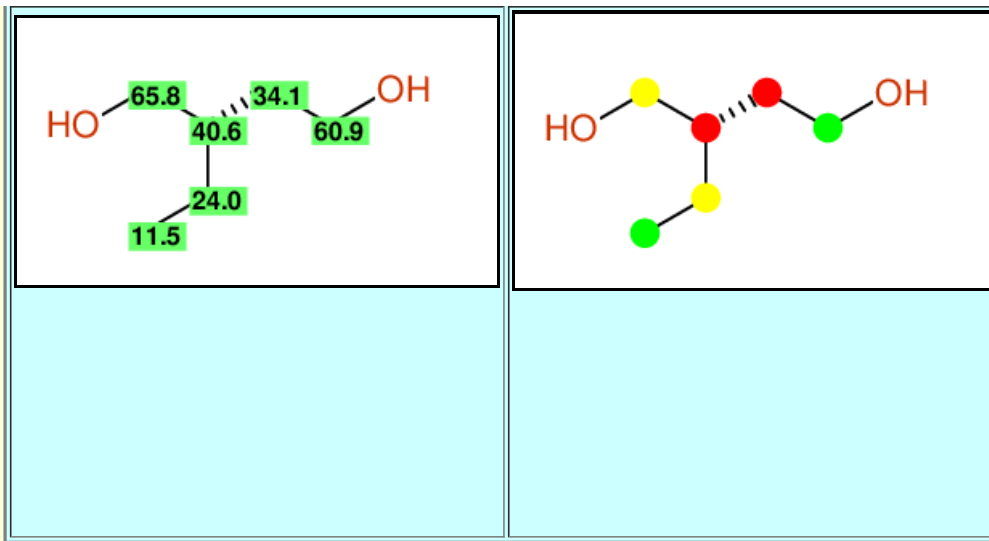
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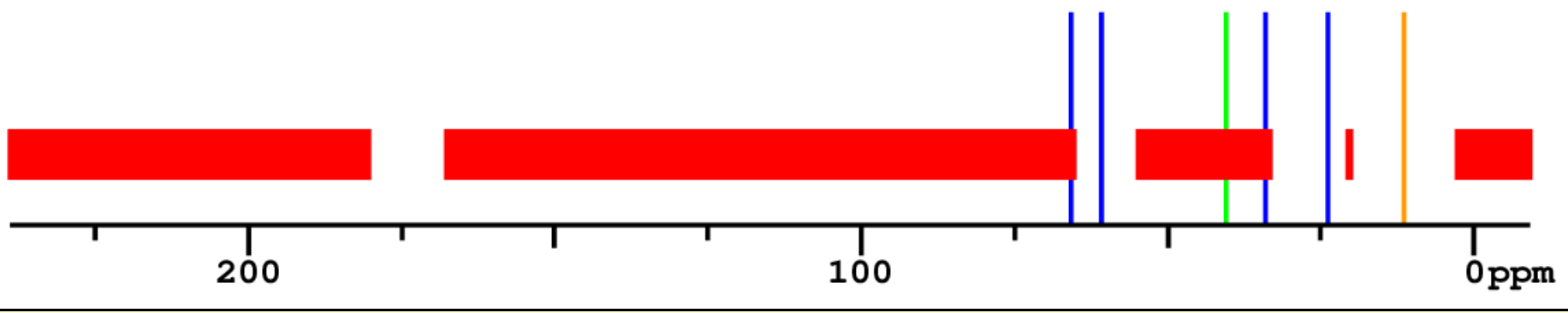
Structure Proposal #26

Structure	Similarity Measure
	<p>Deviation = 4.98 ppm (Different pattern)</p> <p>$C_6H_{14}O_2$</p> <p>MWT = 118.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>CYVMBANVYOZFIG</p>
Predicted Chemical Shiftvalues	Matching Map




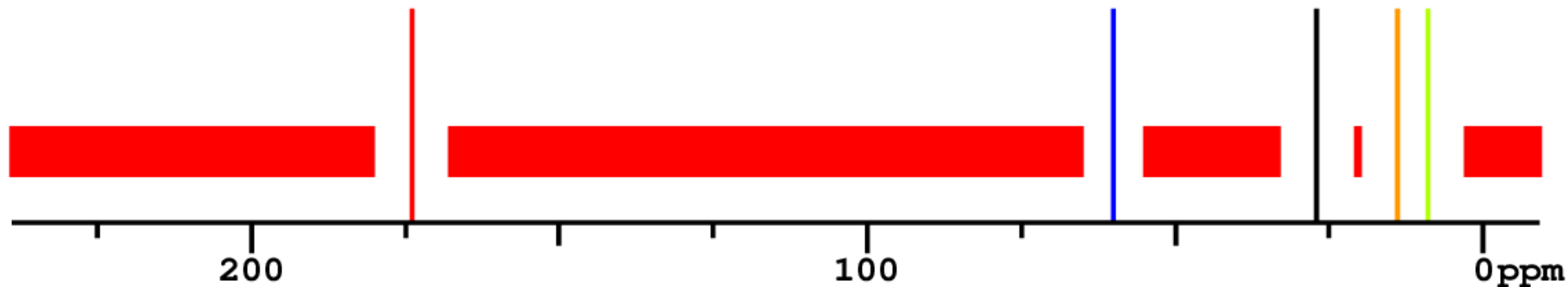
Predicted shift values

Signal multiplicity: S D T Q O E P ?



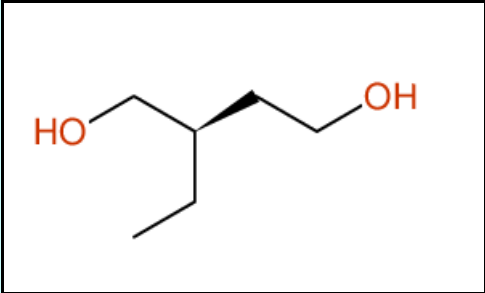
Experimental shift values

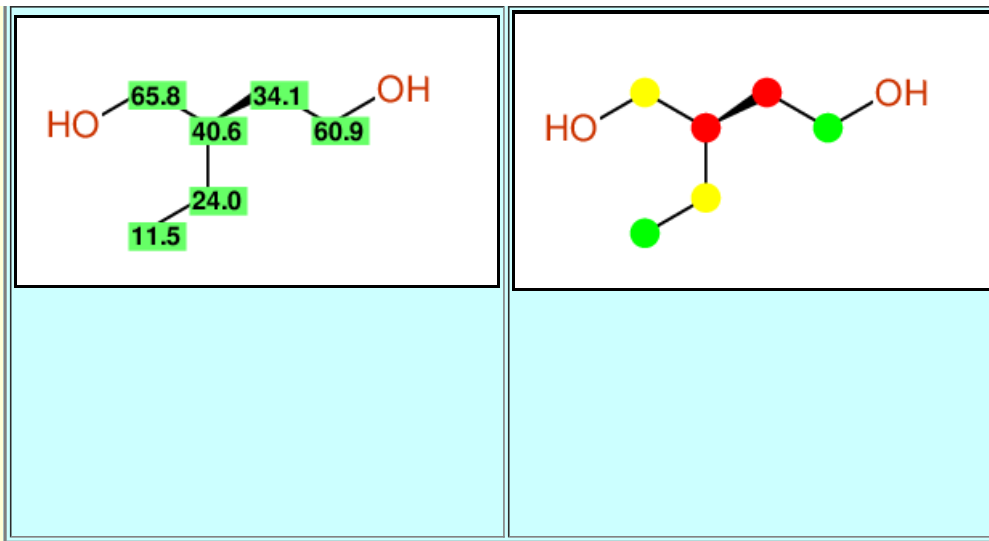
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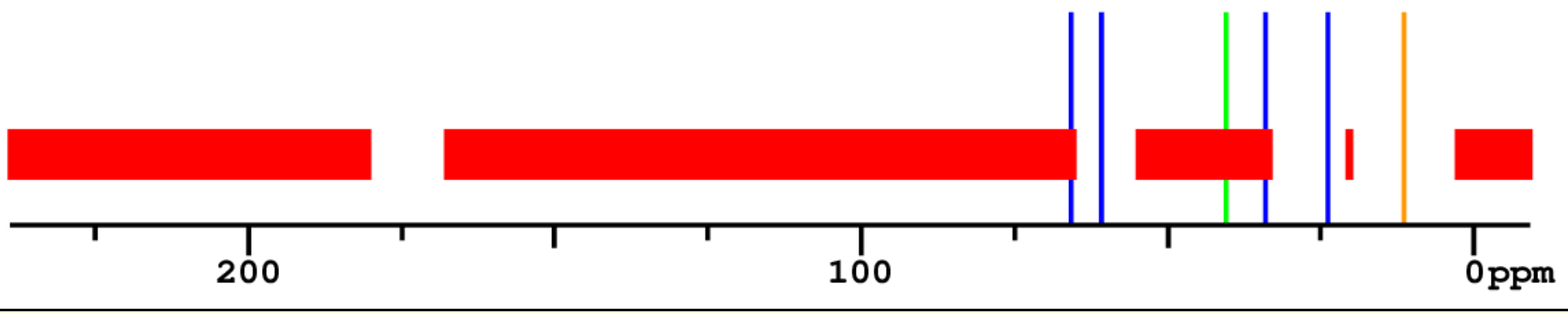
Structure Proposal #27

Structure	Similarity Measure
	<p>Deviation = 4.98 ppm (Different pattern)</p> <p>$C_6H_{14}O_2$</p> <p>MWT = 118.07</p> <p>PUBCHEM</p> <p>Search Web for this structure:</p> <p>CYVMBANVYOZFIG</p>
Predicted Chemical Shiftvalues	Matching Map



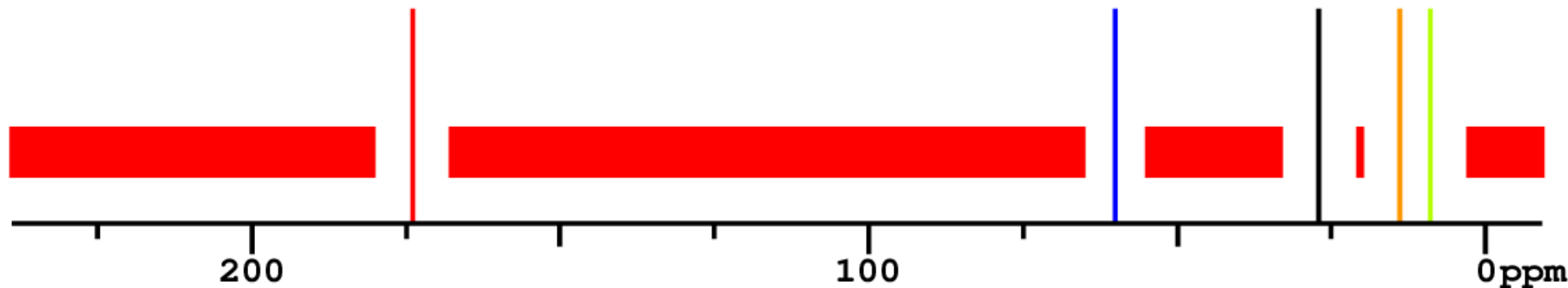
Predicted shift values

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



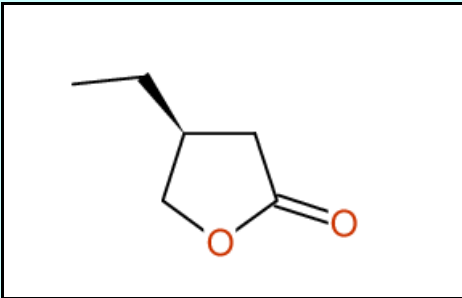
Experimental shift values

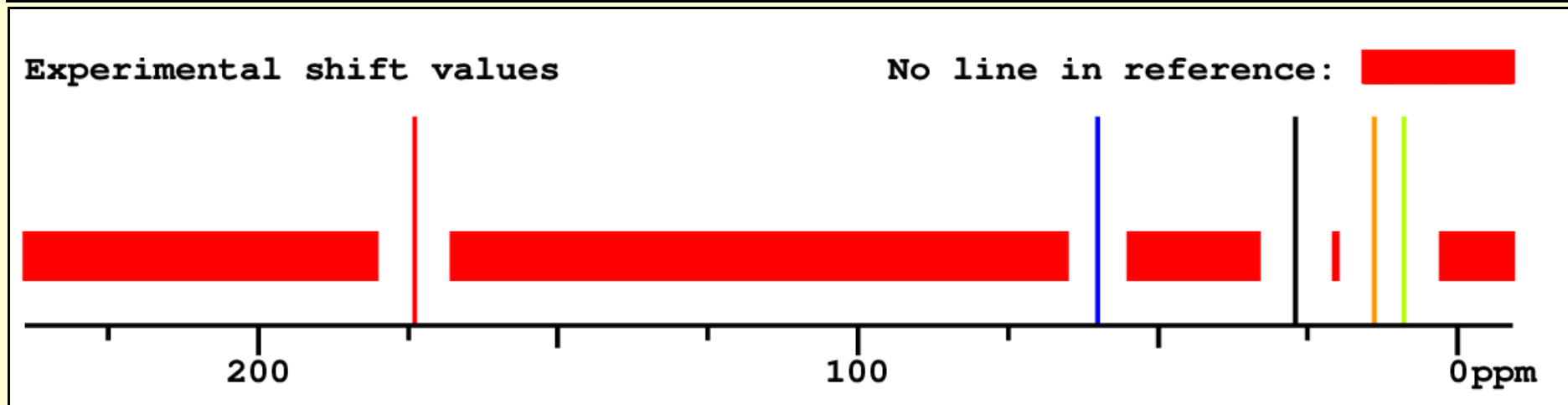
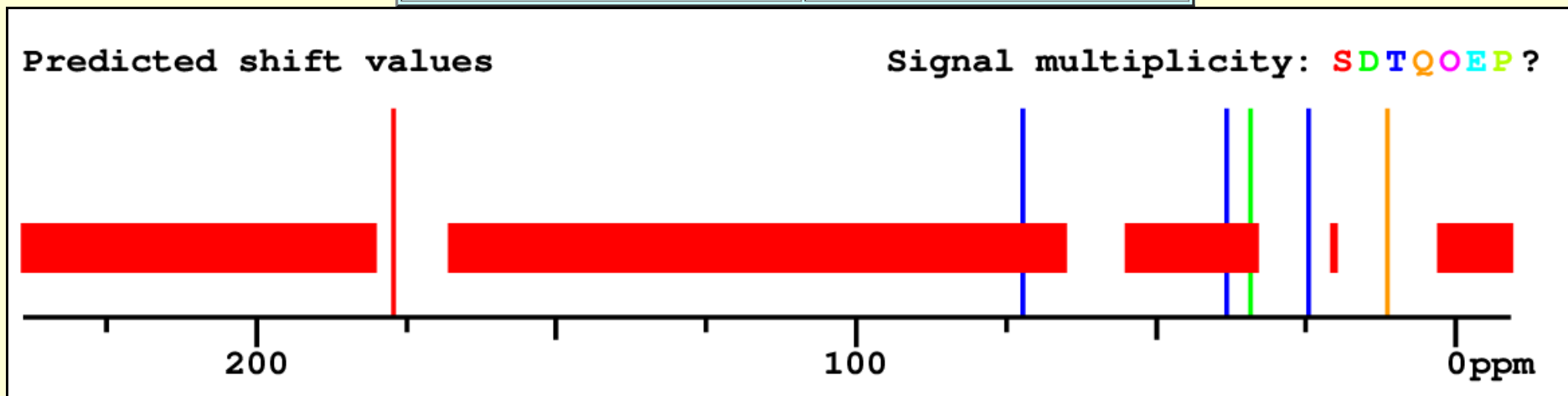
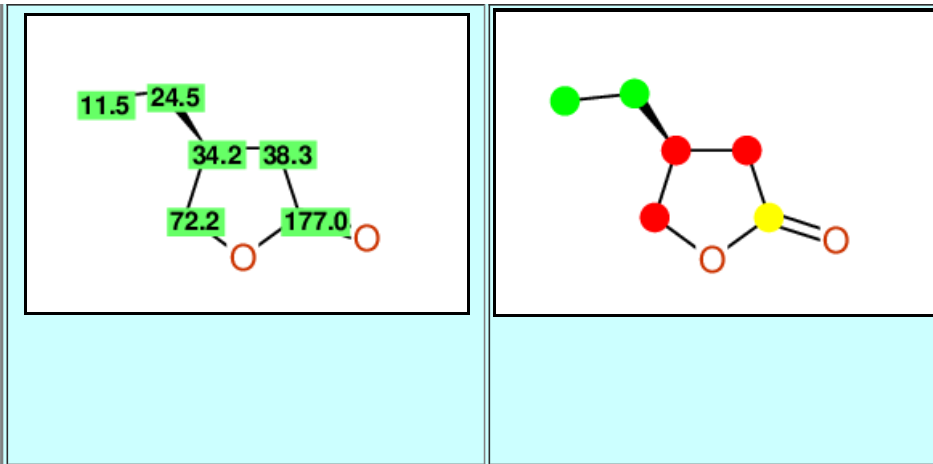
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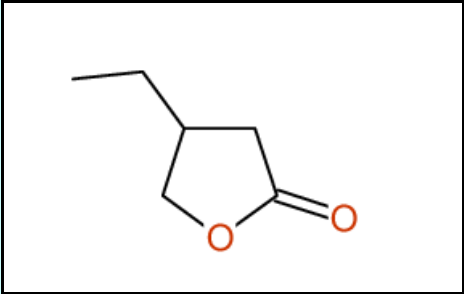
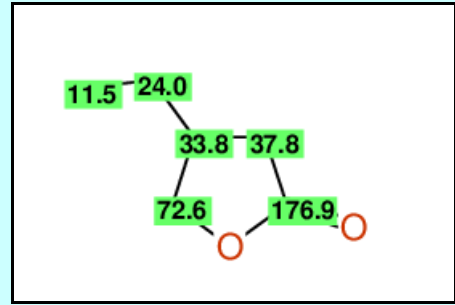
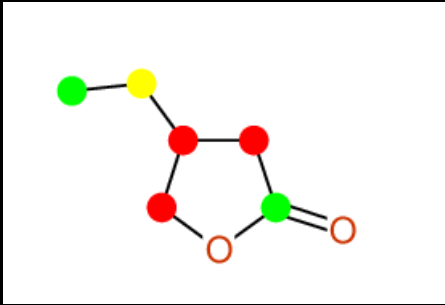
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Structure Proposal #28

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

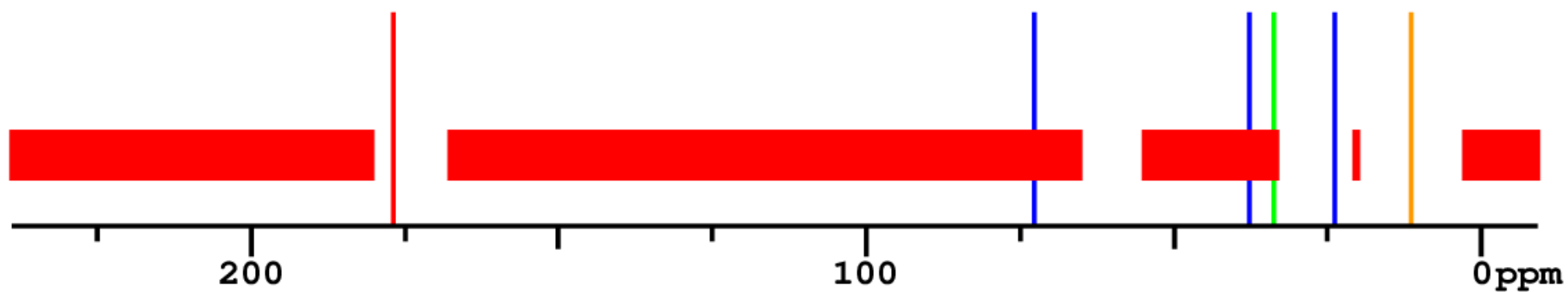


Structure Proposal #29

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
 <p>Chemical structure with predicted chemical shift values (ppm) in green boxes:</p> <ul style="list-style-type: none">11.524.033.837.872.6176.9	 <p>Chemical structure with colored atoms indicating matching map:</p> <ul style="list-style-type: none">Yellow: Ethyl group carbonsRed: Ring carbonsGreen: Ring oxygen and carbonyl oxygen

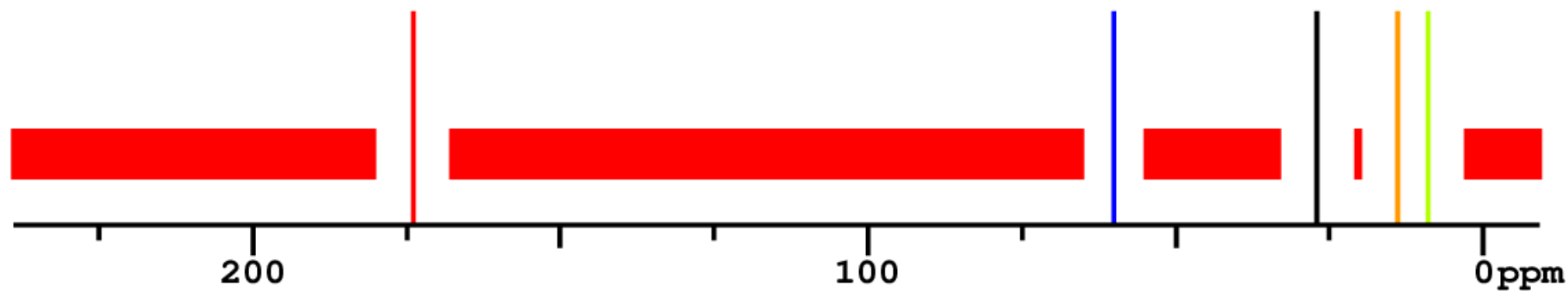
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

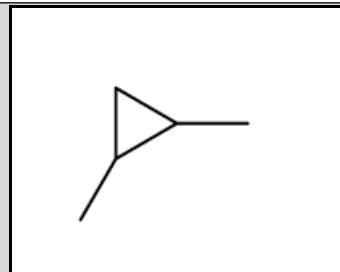


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Summary of the 1 most frequently occurring parent ring systems
within the 27 best-fitting entries

Occurrence:

1 in 27



Summary of Processing

Checking existence of data and counting them:	74,435,185 entries in 0.206 seconds
Applying restraints from elemental composition:	1.761 seconds, 2,773,229 entries remain
Applying restraints from number of signals:	1.946 seconds, 170,467 entries remain
Searching 1,444,403,916 chemical shift values line-per-line:	12.016 seconds
Best 1,562 entries selected for analysis:	2.543 seconds
Ranking of 1,562 entries by similarity:	0.388 seconds
Deviation of best match:	0.87 ppm
Creating table and linking 1,562 structures to 475,803 INCHIKEY-pages:	0.353 seconds
Detailed Analysis of 29 structures including graphical representation:	13.172 seconds
Analysis of 27 structures for common parent ring systems	0.004 seconds
Data transfered from disk:	406 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 19:07

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

Have a nice day !