

**Spectral Similarity Search based on
177,099,966 Structures
downloadable from the INTERNET
using CSEARCH - Technology**

Description of Request

Please cite this service as:

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

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:08

This page will be kept for 30 days here

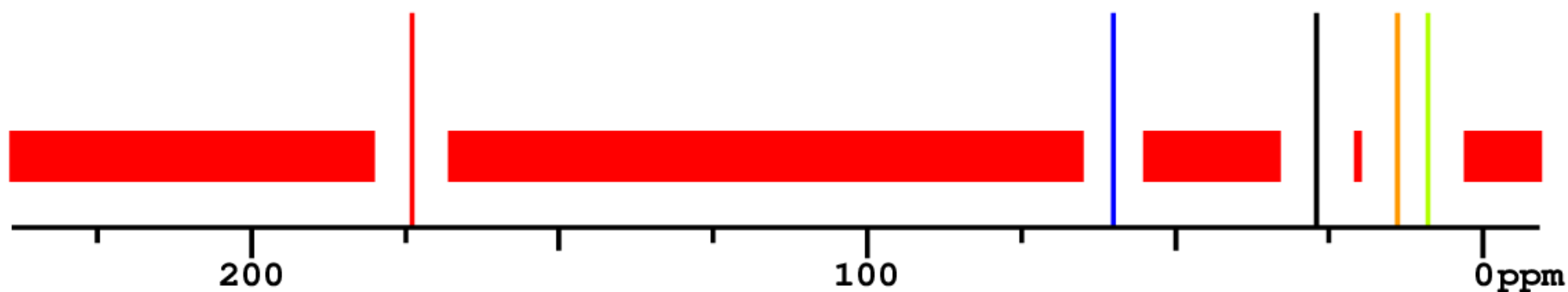
Name of Project:	Test1
Comment:	Dereplication-engine
Name of Compound:	Propionic_acid,ethylester 400MHz

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:	177,099,966
Compounds containing: N	166,999,717
Compounds containing: O	162,430,971
Compounds containing: P	974,070
Compounds containing: S	49,407,848
Compounds containing: F	33,953,039
Compounds containing: Cl	22,177,188
Compounds containing: Br	10,360,390
Compounds containing: I	2,002,129
Compounds containing: other	2,140,679

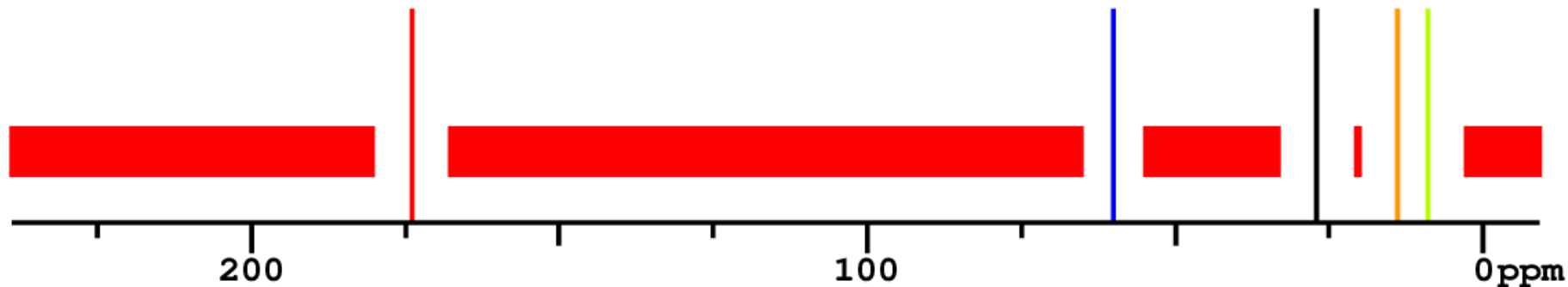
Available entries at each Screening-Step	
Total number of entries:	177,099,966

Applying requested elemental composition:	5,102,397 entries remain
Applying requested number of signals:	218,318 entries remain

Entries per line found out of 218,318 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	S	3.00	26,659	Impurity ?
2	60.00	T	2.50	26,308	Unspecific line
3	27.00	?	3.00	73,749	Unspecific line
4	14.00	Q	3.00	38,183	Impurity ?
5	9.00	P	3.00	29,171	Unspecific line

Experimental shift values

No line in reference: ████████



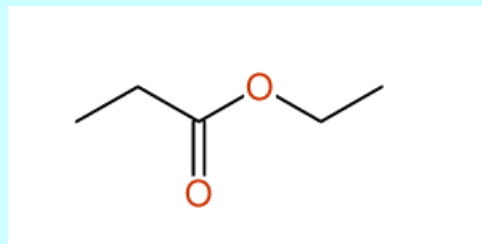
Number of coincident lines versus number of entries		
Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	56	Selected for detailed analysis
4	900	Selected for detailed analysis
3	7,724	Selected for detailed analysis
2	37,724	
1	91,570	

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

0.81 -
0.87ppm

3x found

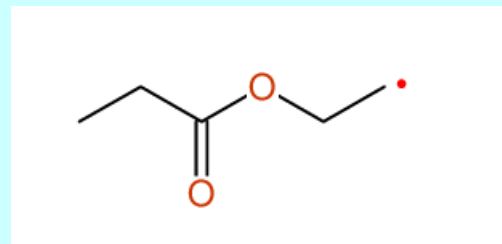
[FKRCODPIKNYEAC](#)



0.81 -
0.81ppm

1x found

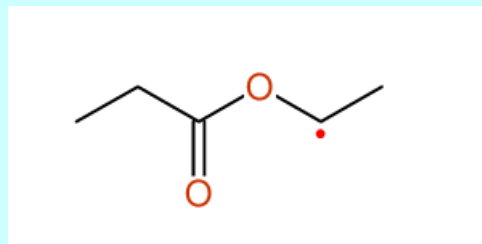
[IRGLFRDZYNBBCO](#)



0.87 -
0.87ppm

1x found

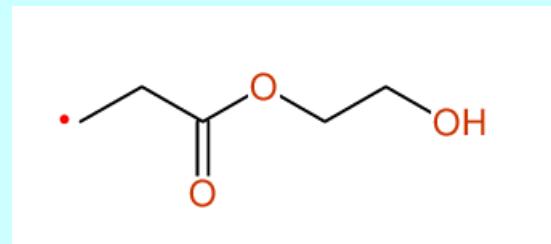
[JLCVJTLAUOPFG](#)



2.02 -
2.02ppm

1x found

[SRWDELNQQOGFGE](#)



2.58 -
2.58ppm

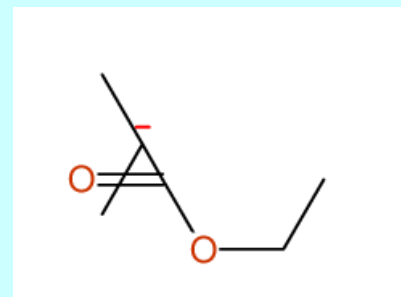
1x found

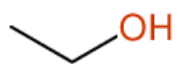
[GZXNSZKTVVWAKU](#)

2.93 -
2.93ppm

1x found

[VNCTWNKFZURVGE](#)

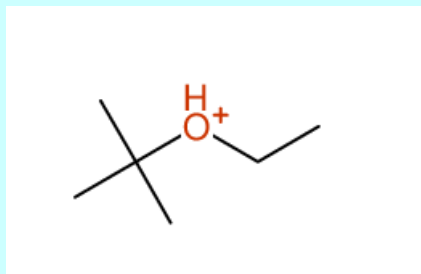




2.99 -
2.99ppm

1x found

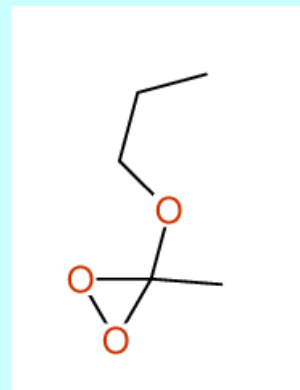
[NUMQCACRALPSHD](#)



2.99 -
2.99ppm

1x found

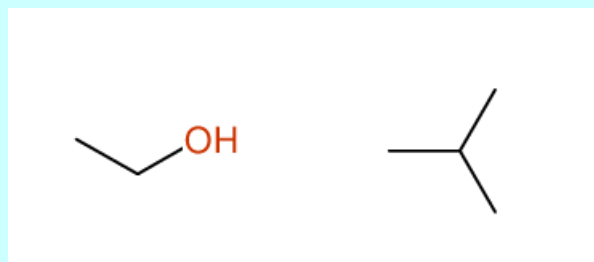
[BZVVMENFRMVWLO](#)



3.07 -
3.07ppm

1x found

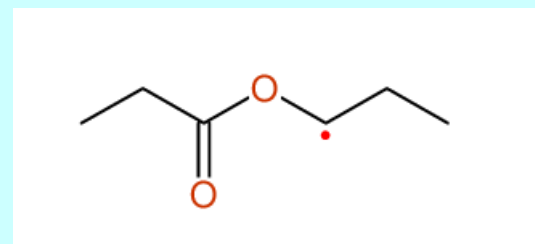
[GSKYFKHLAGYZDU](#)



3.24 -
3.24ppm

1x found

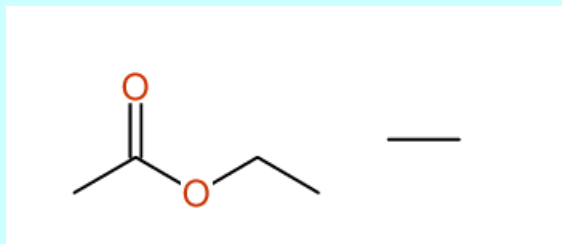
[CDQBJCILHGTWBX](#)



3.27 -
3.27ppm

1x found

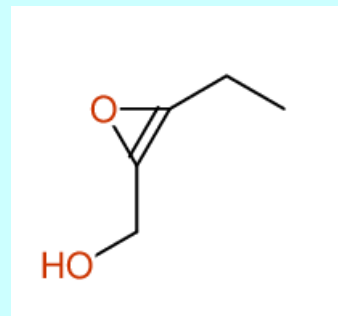
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3.32 -
3.32ppm

1x found

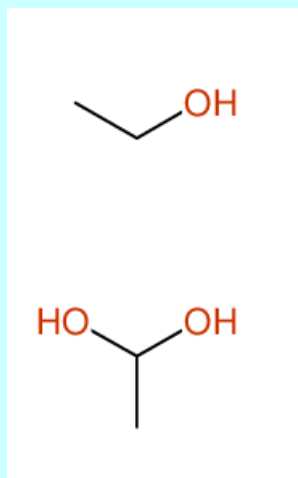
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3.35 -
3.35ppm

1x found

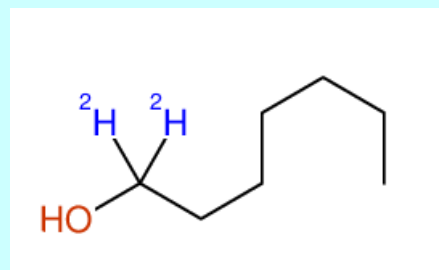
[WLPYHZGVXMAZET](#)



3.38 -
3.38ppm

2x found

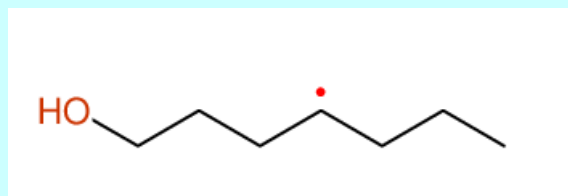
[BBMCTIGTCKYKF](#)



3.38 -
3.38ppm

1x found

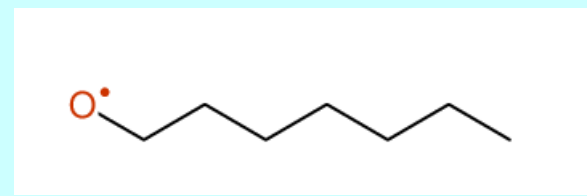
[GORPBXJSOXJRJC](#)



3.38 -
3.38ppm

1x found

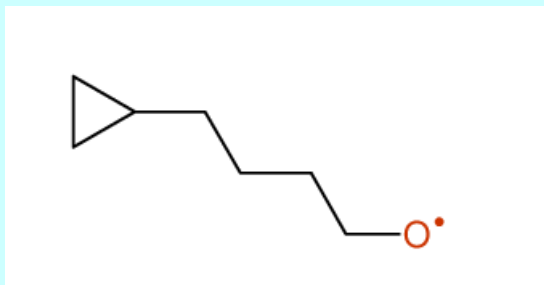
[XBKKJRZFSVTKGZ](#)



3.39 -
3.39ppm

1x found

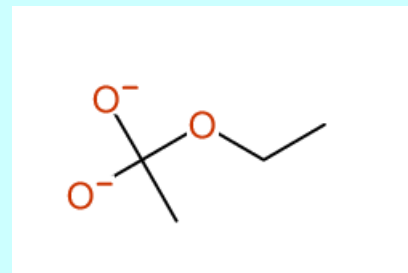
[FRESAHHZYKWMSE](#)



3.40 -
3.40ppm

1x found

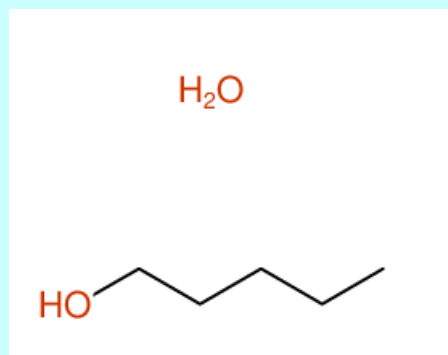
[QNBMMTAJSMBXKY](#)



3.40 -
3.40ppm

1x found

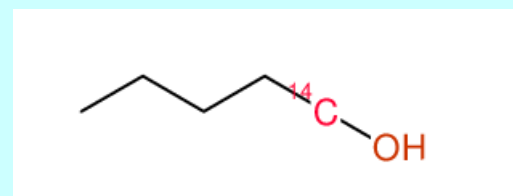
[LBFCRPJWCIHPSX](#)



3.40 -
3.40ppm

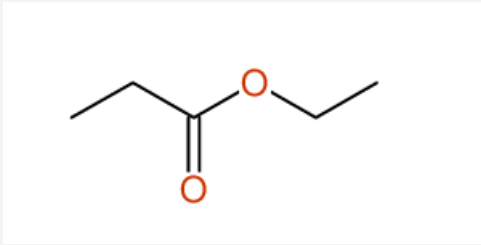

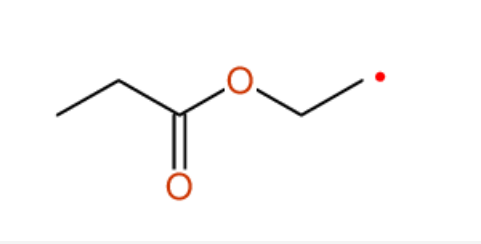
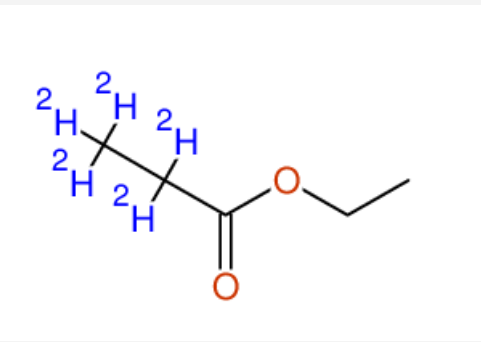

8x found

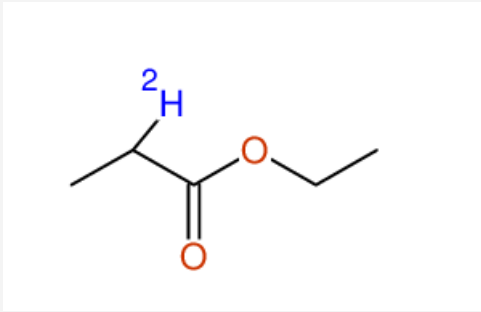

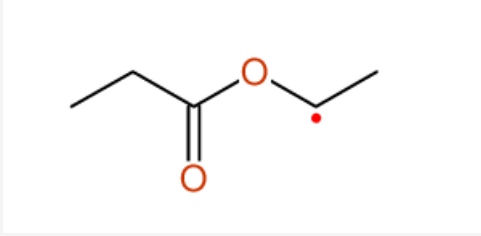
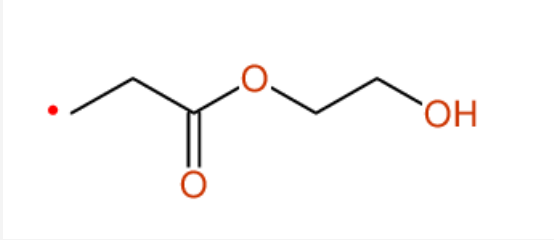
[AMQJEAYHLZJPGS](#)

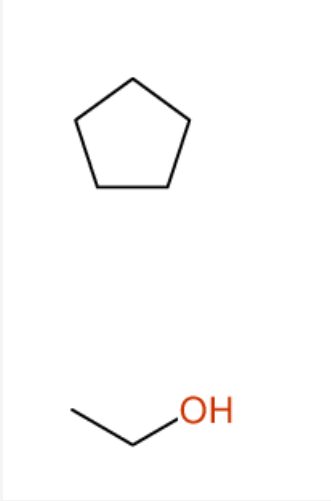
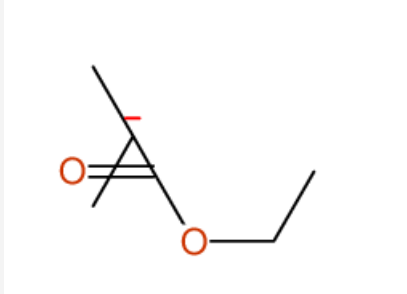
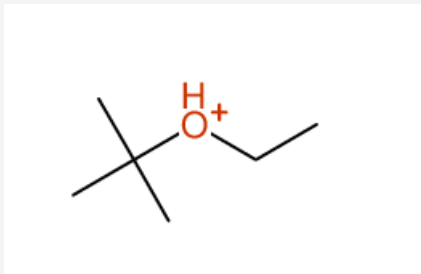



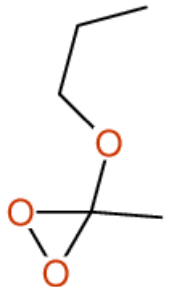

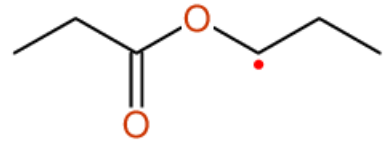
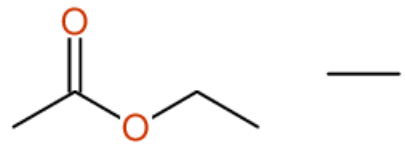
8,680 [Structure proposals](#) found for your C-NMR Spectrum

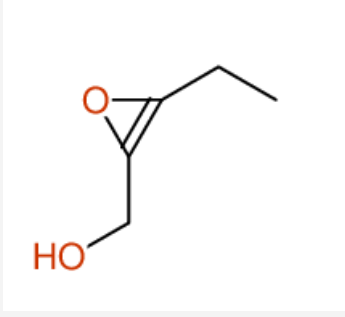
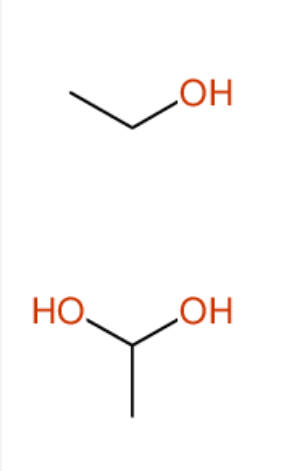
676 Entries will be shown because of your selection of additional constraints

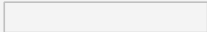

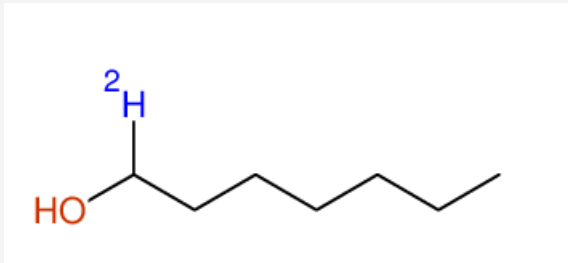

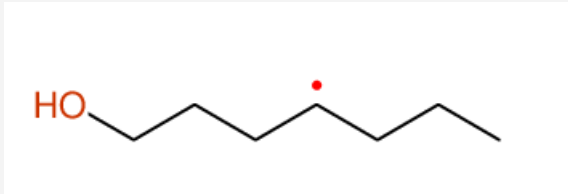
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1 0.81 Details		$C_5H_{10}O_2$ MWT = 102.055	Proposal #1 Structure-ID: 6,776,925 FKRCODPIKNYEAC-IKLDFBCSAQ	Availability of NMR-Data in CSEARCH 
Proposal #2 0.81 Details		$C_5H_9O_2$ MWT = 101.055	Proposal #2 Structure-ID: 6,773,007 IRGLFRDZYNBBCO-IKLDFBCSAI	
Proposal #3 0.87 Details		$C_5H_{10}O_2$ MWT = 107.055	Proposal #3 Structure-ID: 27,004,293 FKRCODPIKNYEAC-WNWXORZEL	Availability of NMR-Data in CSEARCH 

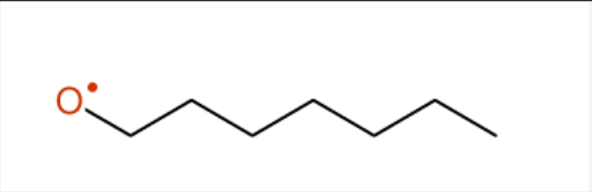
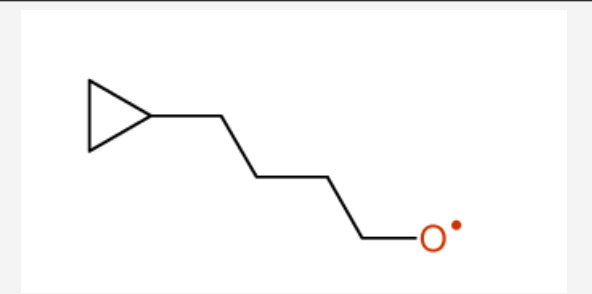
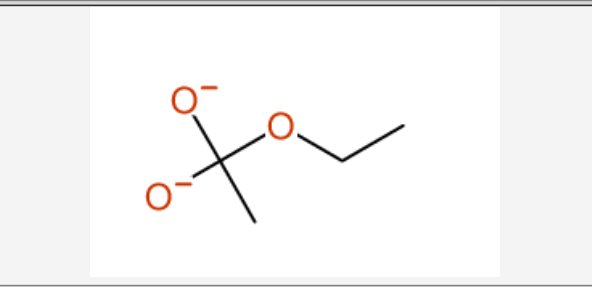
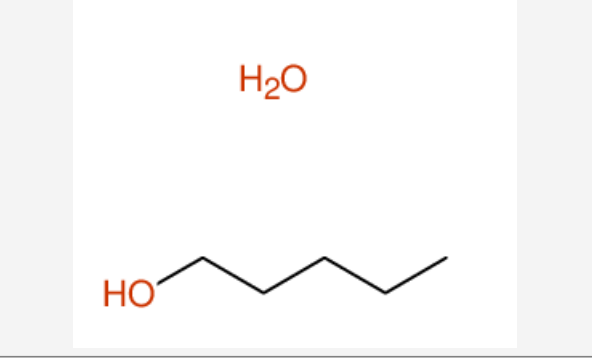
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #4 0.87 Details		$C_5H_{10}O_2$ MWT = 103.055	Proposal #4 Structure-ID: 77,343,682 FKRCODPIKNYEAC-WFVSECRTE	Availability of NMR-Data in CSEARCH 
Proposal #5 0.87 Details		$C_5H_9O_2$ MWT = 101.055	Proposal #5 Structure-ID: 35,970,584 JLCVJT LAUOPPFGE-UHFFFAOYAG	
Proposal #6 2.02 Details		$C_5H_9O_3$ MWT = 117.055	Proposal #6 Structure-ID: 35,385,805 SRWDELNQQOGFGE-UHFFFAOYAC	

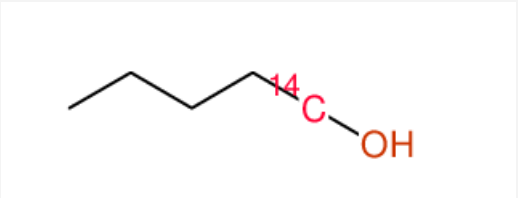

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #7</p> <p>2.58</p> <p>Details</p>	 <p>The diagram shows two chemical structures. The top structure is a five-membered carbon ring (cyclopentane). The bottom structure is ethanol, represented as a two-carbon chain with a hydroxyl group (-OH) attached to the second carbon.</p>	<p>$C_5H_{10} \cdot C_2H_6O$</p> <p>MWT = 116.077</p>	<p>Proposal #7</p> <p>Structure-ID: 2,204,115</p> <p>GZXNSZKTVVWAKU-UHFFFAOYAC</p>	
<p>Proposal #8</p> <p>2.93</p> <p>Details</p>	 <p>The diagram shows a cyclopropane ring with a carboxylate group (-COO-) attached to one of the carbons. The ethyl group (-CH2CH3) is attached to the oxygen atom of the carboxylate group, forming ethyl cyclopropanecarboxylate.</p>	<p>$C_6H_{11}O_2$</p> <p>MWT = 115.066</p>	<p>Proposal #8</p> <p>Structure-ID: 132,225,892</p> <p>VNCTWNKFZURVGF-UHFFFAOYAA</p>	
<p>Proposal #9</p> <p>2.99</p> <p>Details</p>	 <p>The diagram shows a tert-butyl group (a central carbon bonded to three methyl groups) connected to an oxygen atom, which is further connected to an ethyl group (-CH2CH3). This represents ethyl tert-butyl ether.</p>	<p>$C_6H_{14}O$</p> <p>MWT = 102.066</p>	<p>Proposal #9</p> <p>Structure-ID: 42,729,330</p> <p>NUMQCACRALPSHD-IKLDfBCSAV</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #10 2.99 Details		$C_5H_{10}O_3$ MWT = 118.055	Proposal #10 Structure-ID: 157,519,640 BZVVMENFRMVWLO-UHFFFAOYAS	
Proposal #11 3.07 Details		$C_4H_{10}.C_2H_6O$ MWT = 104.066	Proposal #11 Structure-ID: 33,202,161 GSKYFKHLAGYZDU-UHFFFAOYAA	
Proposal #12 3.24 Details Different pattern		$C_6H_{11}O_2$ MWT = 115.066	Proposal #12 Structure-ID: 35,805,679 CDQBJCILHGTWBX-UHFFFAOYAT	
Proposal #13 3.27 Details Different pattern		$C_4H_8O_2.C_2H_6$ MWT = 118.066	Proposal #13 Structure-ID: 12,183,409 ZRKANPPNISQQGA-UHFFFAOYAP	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #14</p> <p>3.32</p> <p>Details</p>		<p>$C_5H_8O_2$</p> <p>MWT = 100.055</p>	<p>Proposal #14</p> <p>Structure-ID: 148,758,066</p> <p>ZZJKPPUKODAOML-UHFFFAOYAI</p>	
<p>Proposal #15</p> <p>3.35</p> <p>Details</p>		<p>$C_2H_6O_2 \cdot C_2H_6O$</p> <p>MWT = 108.044</p>	<p>Proposal #15</p> <p>Structure-ID: 25,364,152</p> <p>WLPYHZGVXMAZET-UHFFFAOYAD</p>	

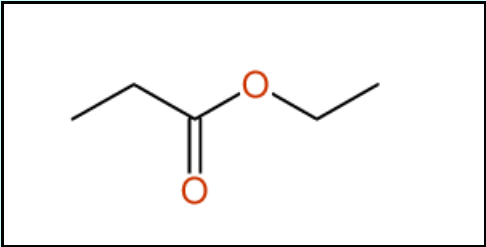
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #16 3.38 Details Different pattern		$C_7H_{16}O$ MWT = 118.077	Proposal #16 Structure-ID: 124,626,008 BBMCTIGTTCKYKF-RJSZUWSAEW	Availability of NMR-Data in CSEARCH 
Proposal #17 3.38 Details Different pattern		$C_7H_{16}O$ MWT = 117.077	Proposal #17 Structure-ID: 114,905,832 BBMCTIGTTCKYKF-WHRKIXHSEV	Availability of NMR-Data in CSEARCH 
Proposal #18 3.38 Details Different pattern		$C_7H_{15}O$ MWT = 115.077	Proposal #18 Structure-ID: 28,025,255 GORPBXJSOXJRJC-UHFFFAOYAM	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #19 3.38 Details Different pattern		$C_7H_{15}O$ MWT = 115.077	Proposal #19 Structure-ID: 35,233,466 XBKKJRZFSVTKGZ-UHFFFAOYAW	
Proposal #20 3.39 Details Different pattern		$C_7H_{13}O$ MWT = 113.077	Proposal #20 Structure-ID: 28,046,870 FRESAHZYKWMSE-UHFFFAOYAM	
Proposal #21 3.40 Details		$C_4H_8O_3$ MWT = 104.044	Proposal #21 Structure-ID: 24,892,999 QNBMMTAJSMBXKY-UHFFFAOYAF	
Proposal #22 3.40 Details	H_2O 	$C_5H_{12}O \cdot H_2O$ MWT = 106.055	Proposal #22 Structure-ID: 25,783,103 LBFCRPJWCIHPSX-UHFFFAOYAI	

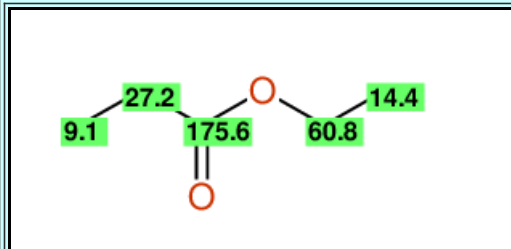
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #23</p> <p>3.40</p> <p>Details</p>		<p>$C_5H_{12}O$</p> <p>MWT = 90.055</p>	<p>Proposal #23</p> <p>Structure-ID: 10,360,545</p> <p>AMQJEAYHLZJPGS-RHRFEJLCER</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Detailed Analysis

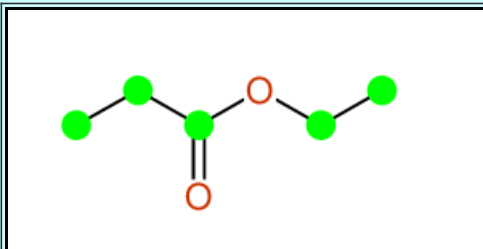
Structure Proposal #1

Structure	Similarity Measure
	<p>Deviation = 0.81 ppm Similarity = 100 %</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 102.06</p> <p>Search Web for this structure:</p> <p>FKRCODPIKNYEAC</p> <p>Availability</p>

Predicted Chemical Shiftvalues

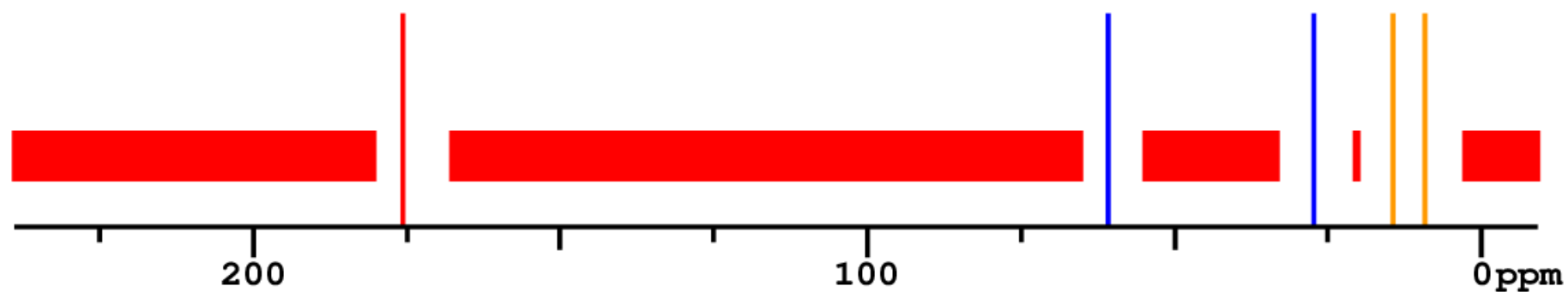


Matching Map



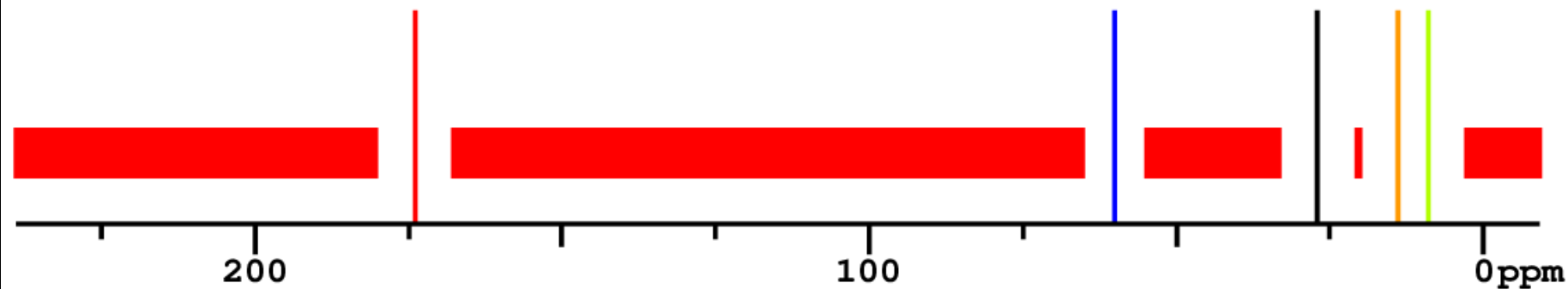
Predicted shift values

Signal multiplicity: S D T Q O E P ?

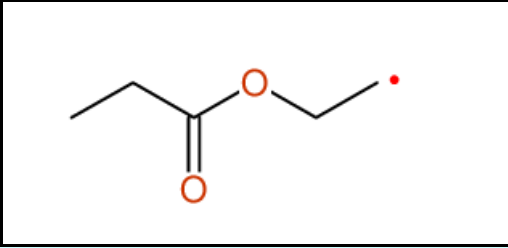
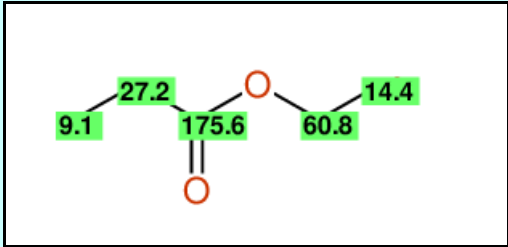
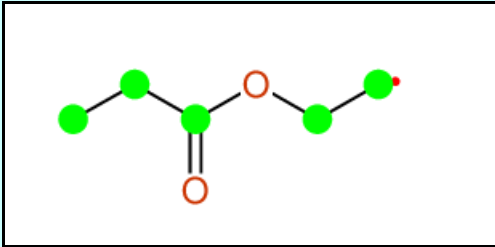


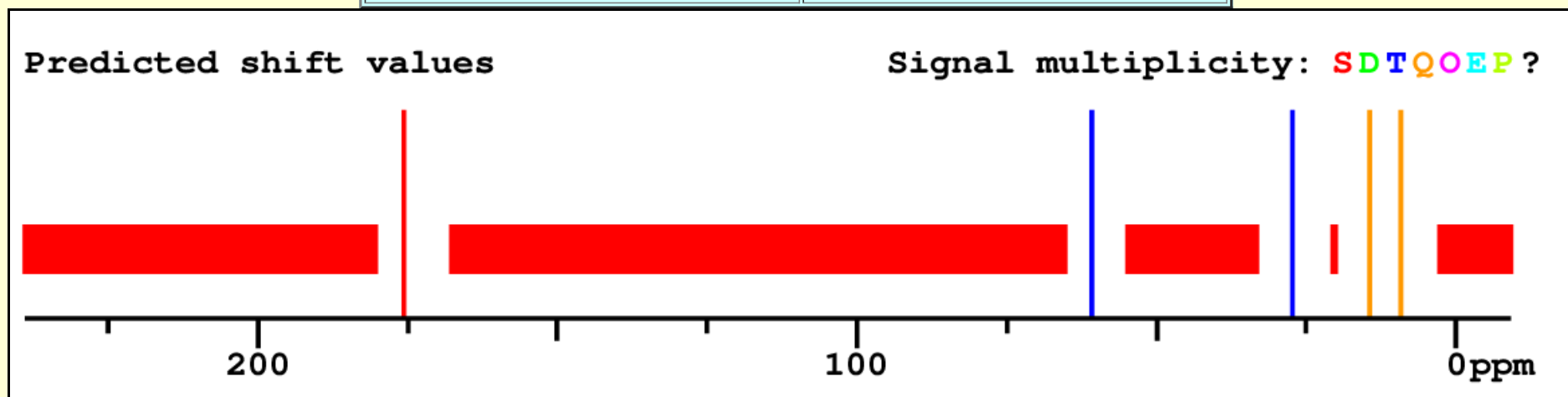
Experimental shift values

No line in reference:



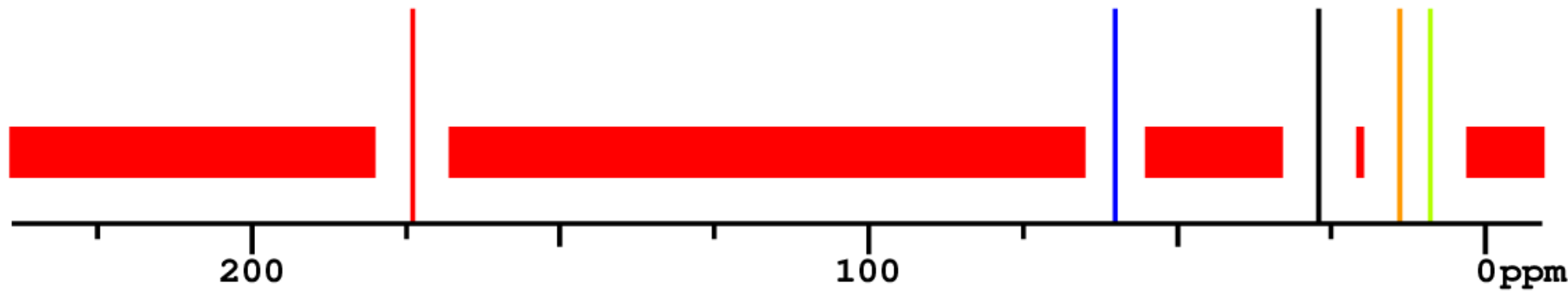
Structure Proposal #2

Structure	Similarity Measure
	Deviation = 0.81 ppm Similarity = 100 % $C_5H_{10}O_2$ MWT = 101.06 Search Web for this structure: IRGLFRDZYNBBCO
Predicted Chemical Shiftvalues	Matching Map
	



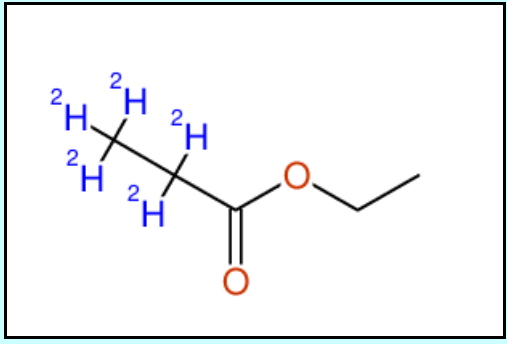
Experimental shift values

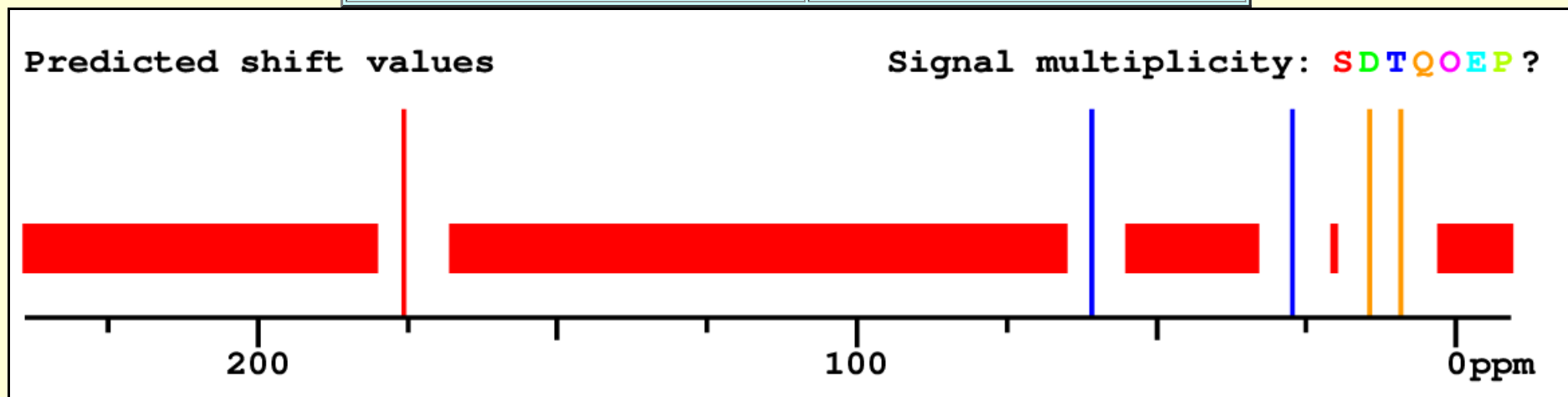
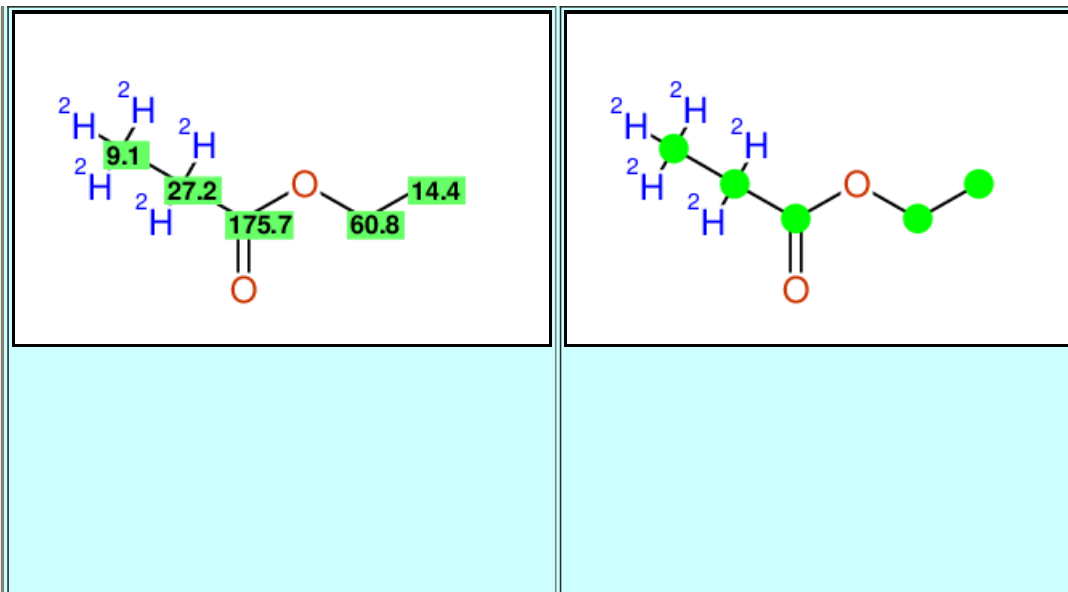
No line in reference: 



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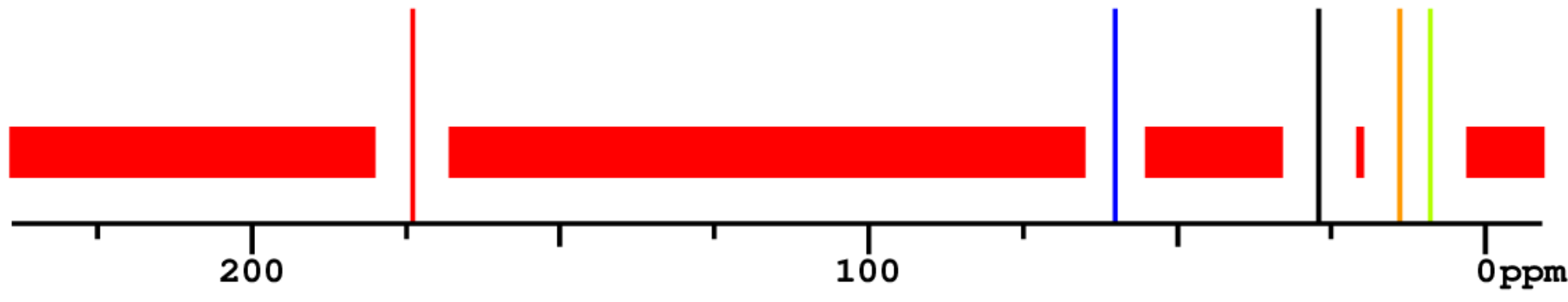
Structure Proposal #3

Structure	Similarity Measure
 <p>The chemical structure shows ethyl propyl carboxylate, <chem>CCCC(=O)OCC</chem>. The hydrogen atoms on the propyl chain are labeled with the number '2', indicating their multiplicity in the NMR spectrum.</p>	<p>Deviation = 0.87 ppm Similarity = 100 %</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 107.06</p> <p>Search Web for this structure: FKRCODPIKNYEAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



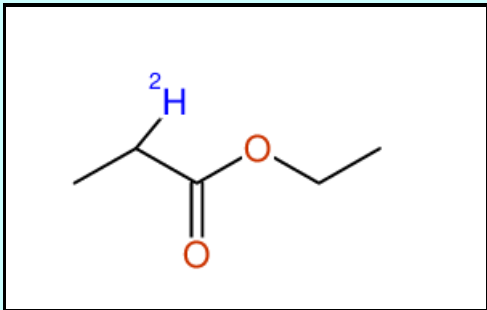
Experimental shift values

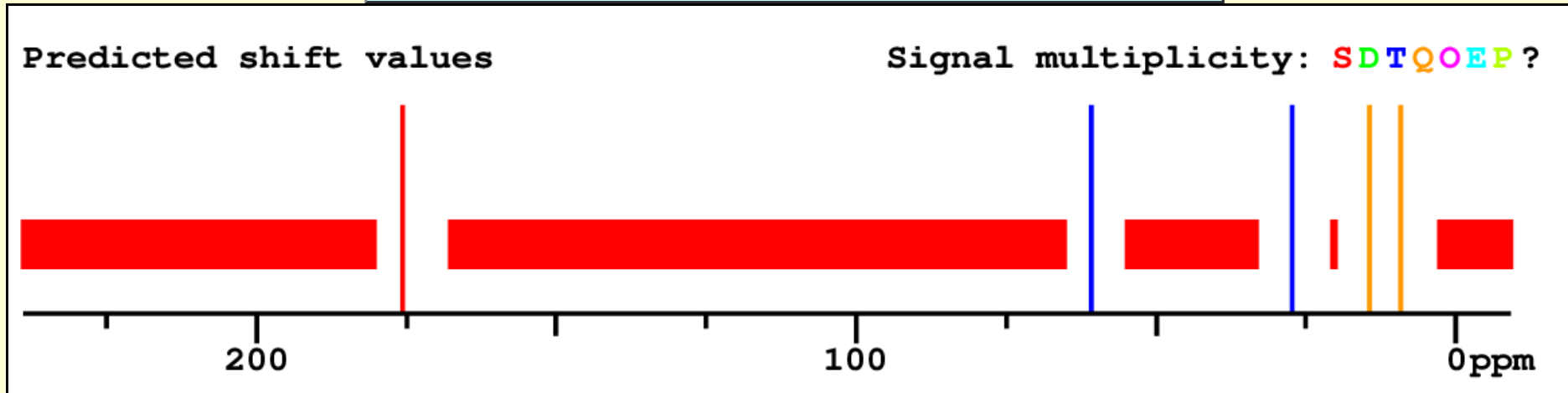
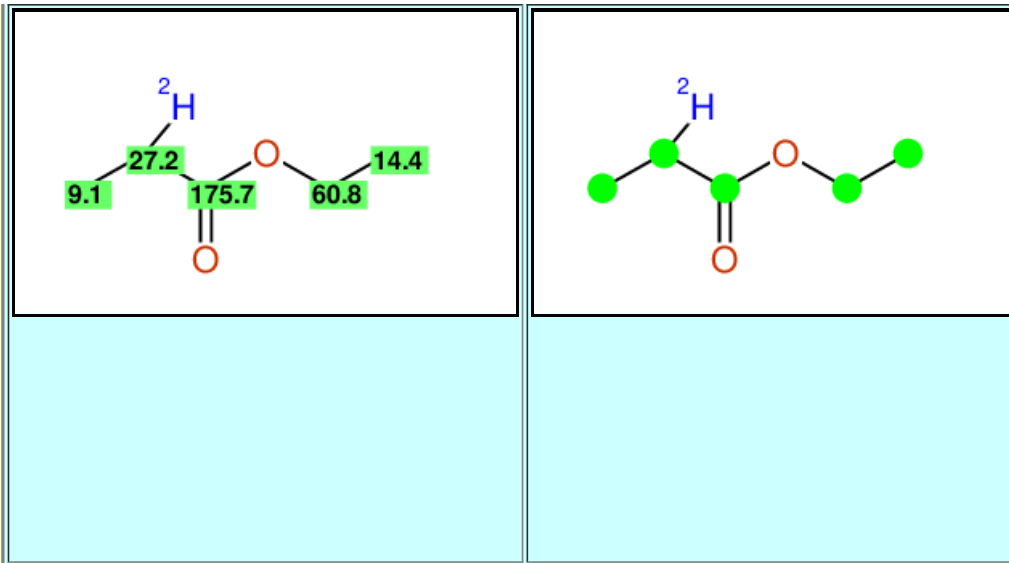
No line in reference: 



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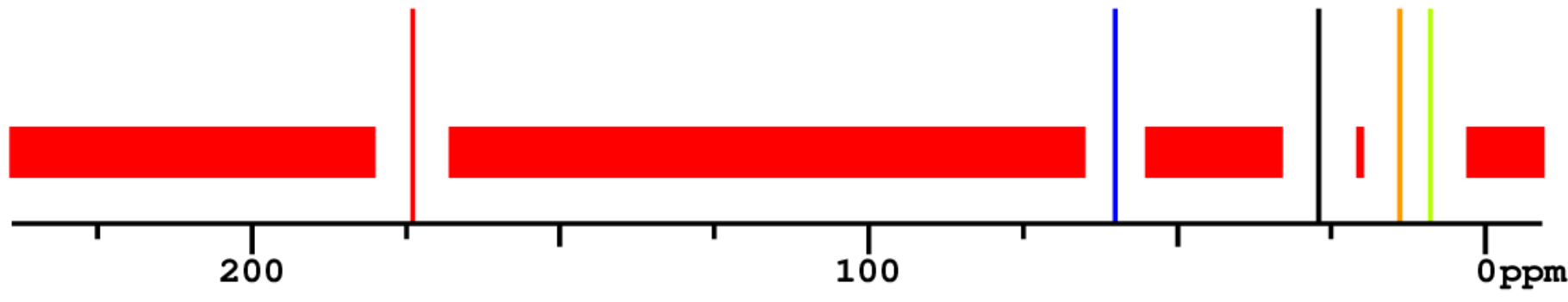
Structure Proposal #4

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm Similarity = 100 %</p> <p>$C_5H_{10}O_2$</p> <p>MWT = 103.06</p> <p>Search Web for this structure: FKRCODPIKNYEAC</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



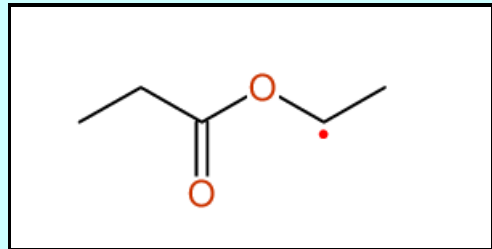
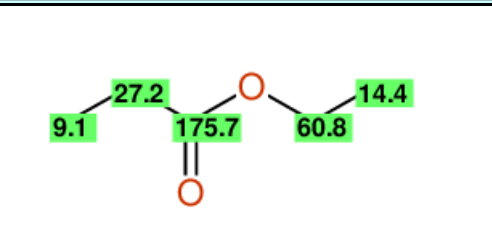
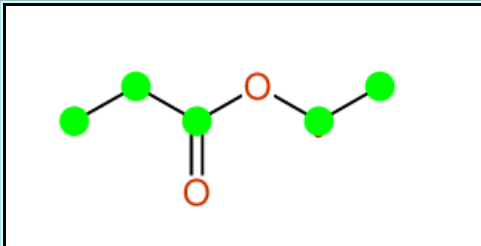
Experimental shift values

No line in reference: 



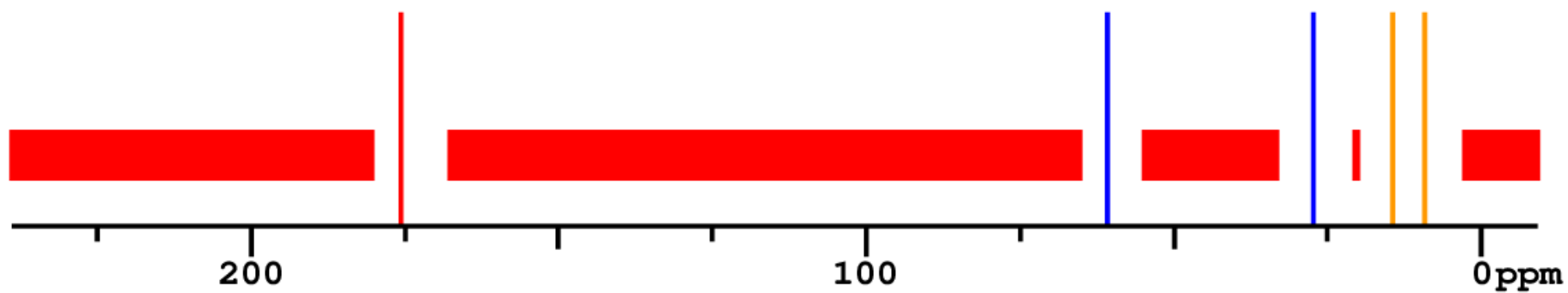
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Structure Proposal #5

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm Similarity = 100 %</p> <p>$C_5H_{10}O$</p> <p>MWT = 101.06</p> <p>Search Web for this structure: JLCVJTLAUOPPEG</p>
Predicted Chemical Shiftvalues	Matching Map
	

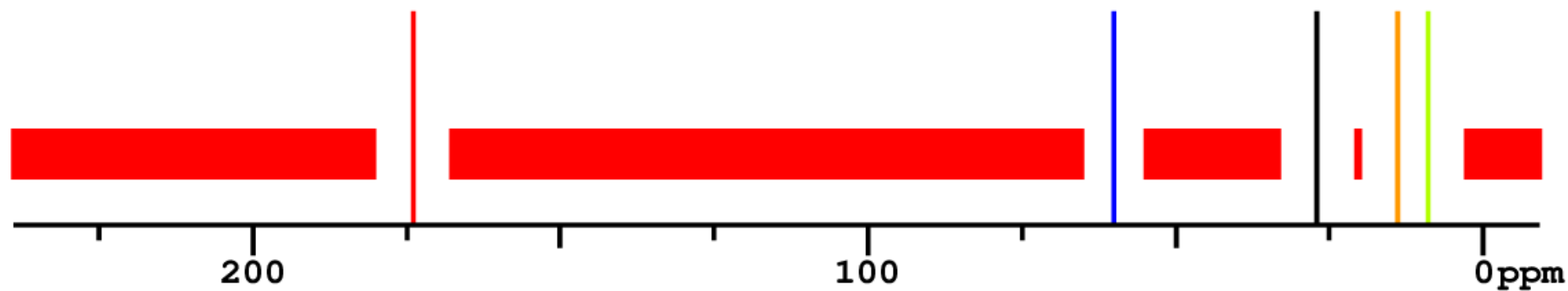
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

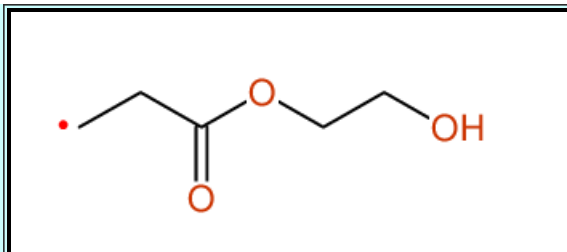
No line in reference: [red bar]



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Structure Proposal #6

Structure	Similarity Measure



Deviation = 2.02 ppm
Similarity = 90 %

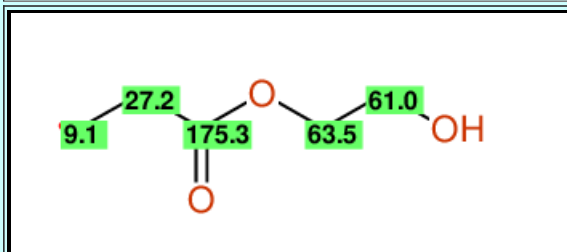
$C_5H_9O_3$

MWT = 117.06

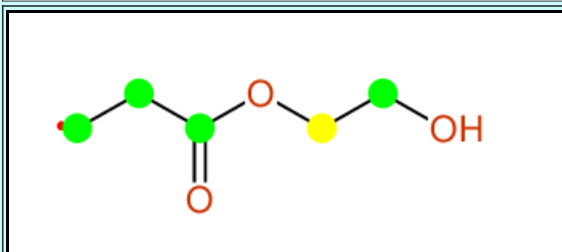
Search Web for this structure:

[SRWDELNQOGFGE](#)

Predicted Chemical Shiftvalues

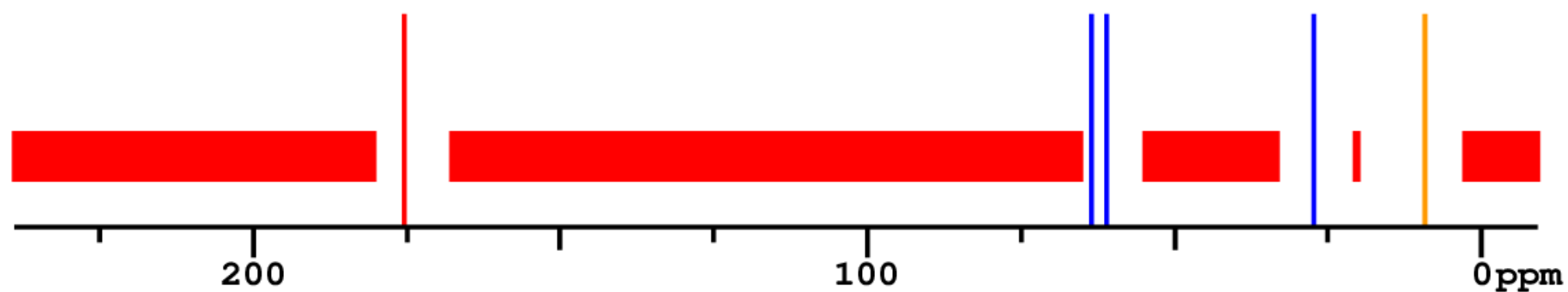


Matching Map



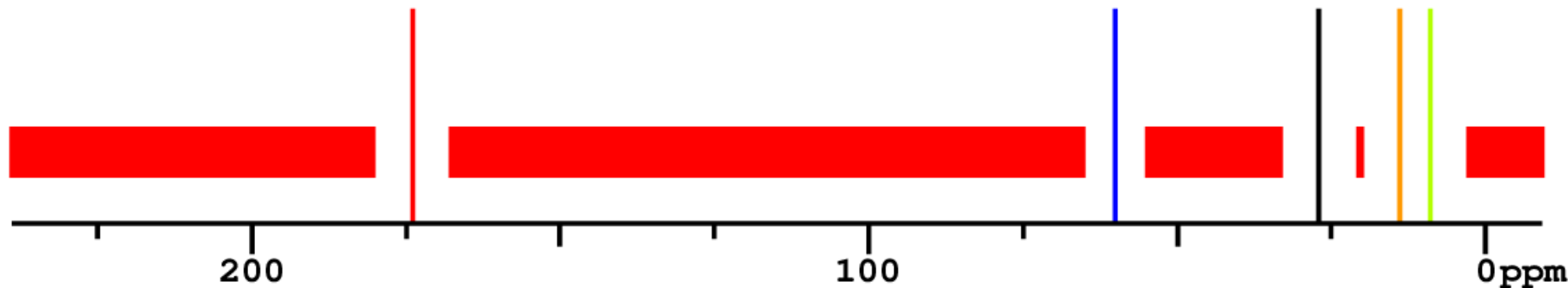
Predicted shift values

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



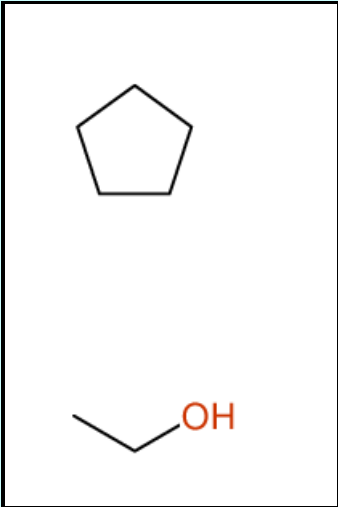
Experimental shift values

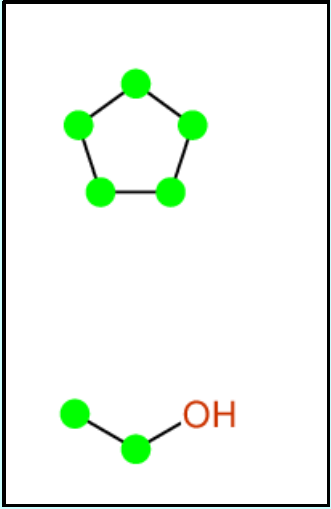
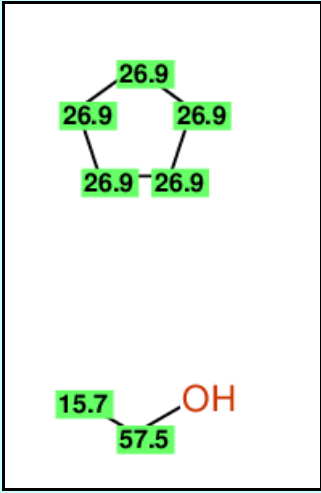
No line in reference: 



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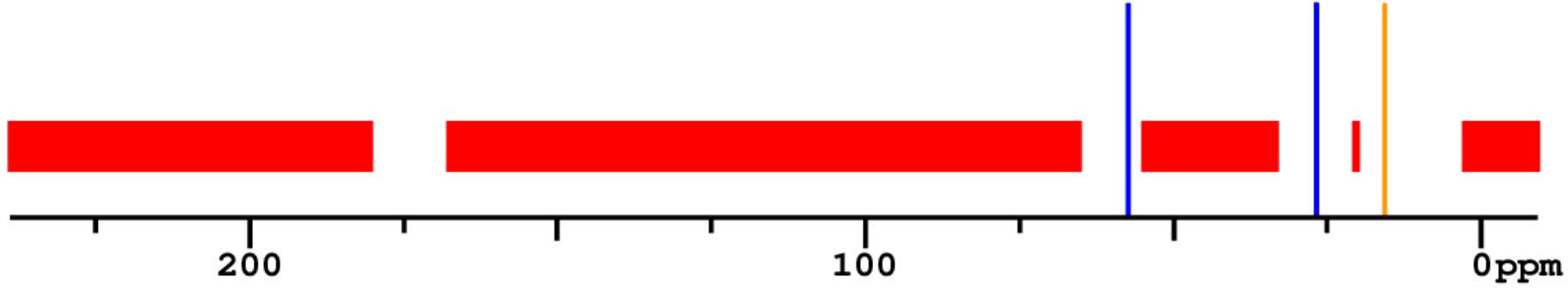
Structure Proposal #7

Structure	Similarity Measure
 <p>The structure shows a five-membered carbon ring (cyclopentane) with a hydroxyl group (-OH) attached to one of the carbons. The OH group is drawn in red.</p>	<p>Deviation = 2.58 ppm Similarity = 100 %</p> <p>$C_5H_{10}O$</p> <p>MWT = 116.08</p> <p>Search Web for this structure: GZXNSZKTVVWAKU</p>
Predicted Chemical Shiftvalues	Matching Map



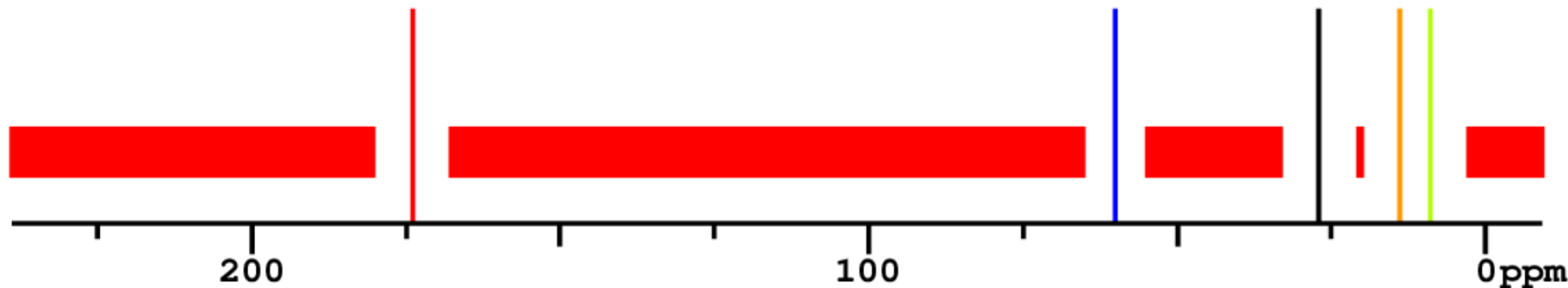
Predicted shift values

Signal multiplicity: S D T Q O E P ?



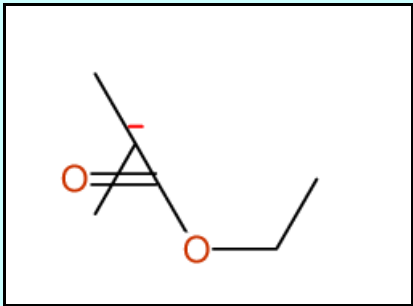
Experimental shift values

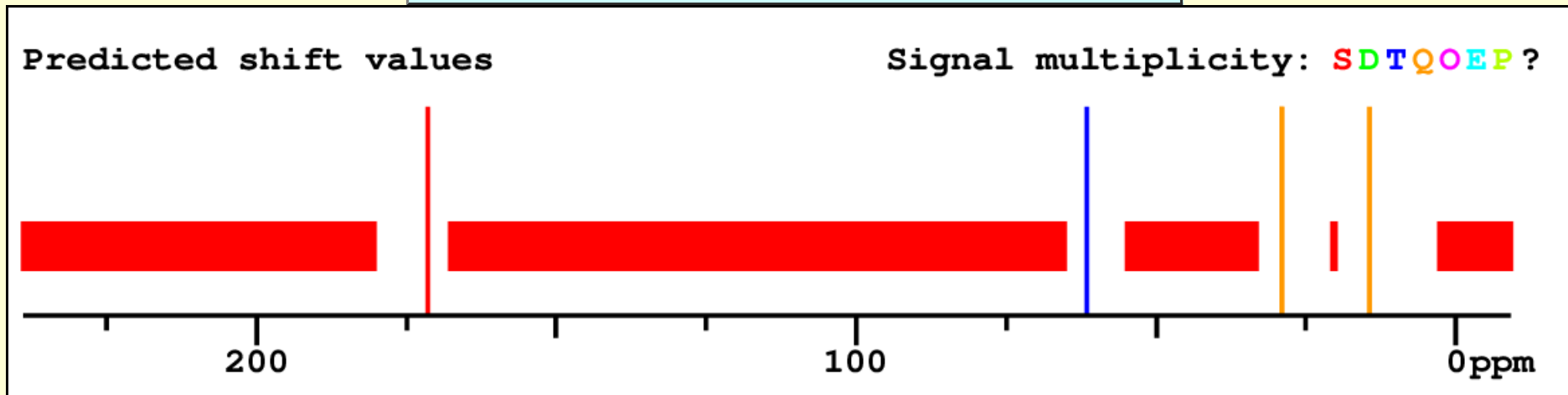
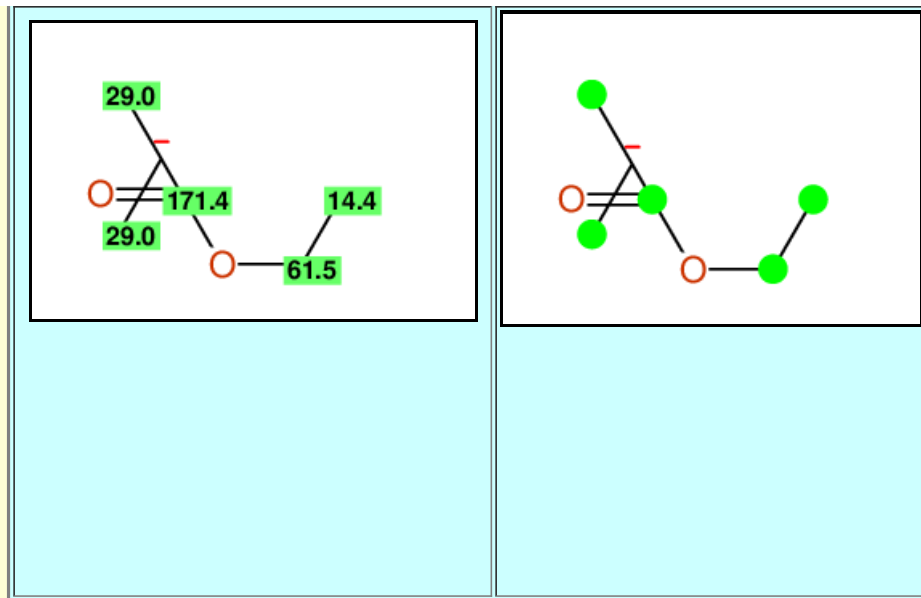
No line in reference: 



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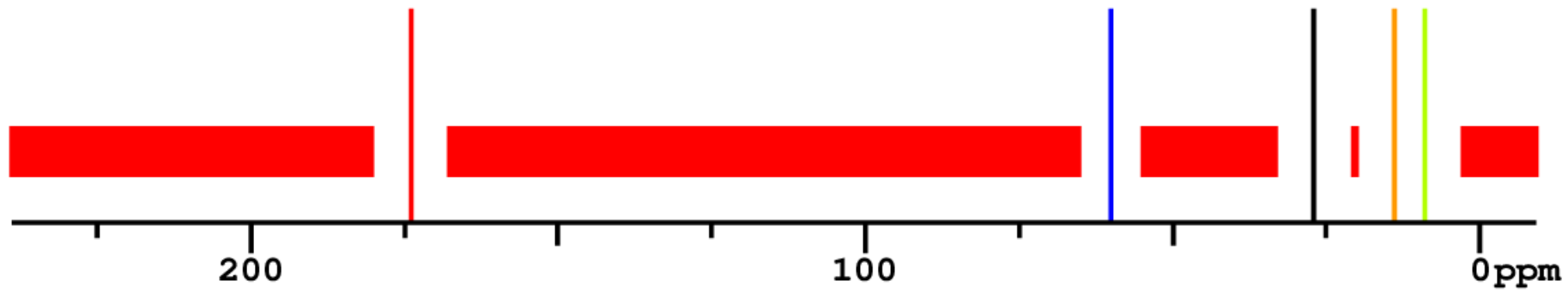
Structure Proposal #8

Structure	Similarity Measure
	Deviation = 2.93 ppm Similarity = 100 % $C_6H_{11}O_2$ MWT = 115.07 Search Web for this structure: VNCTWNKFZURVGE
Predicted Chemical Shiftvalues	Matching Map



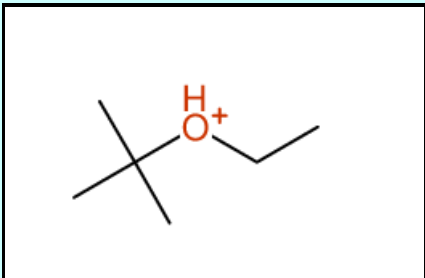
Experimental shift values

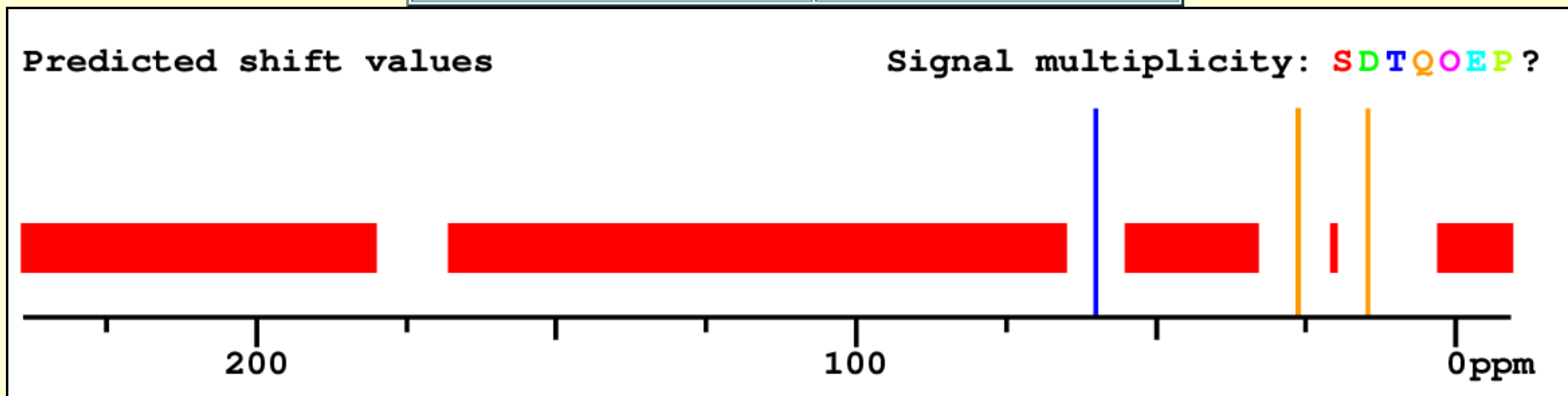
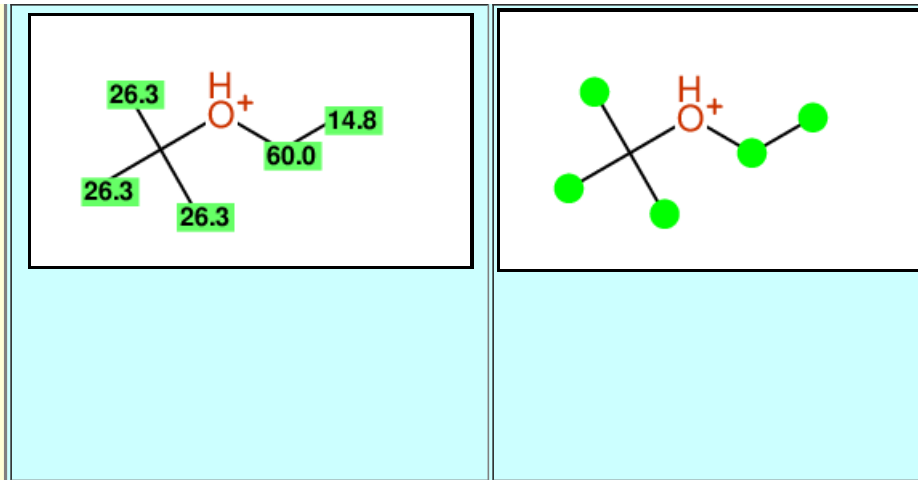
No line in reference: 



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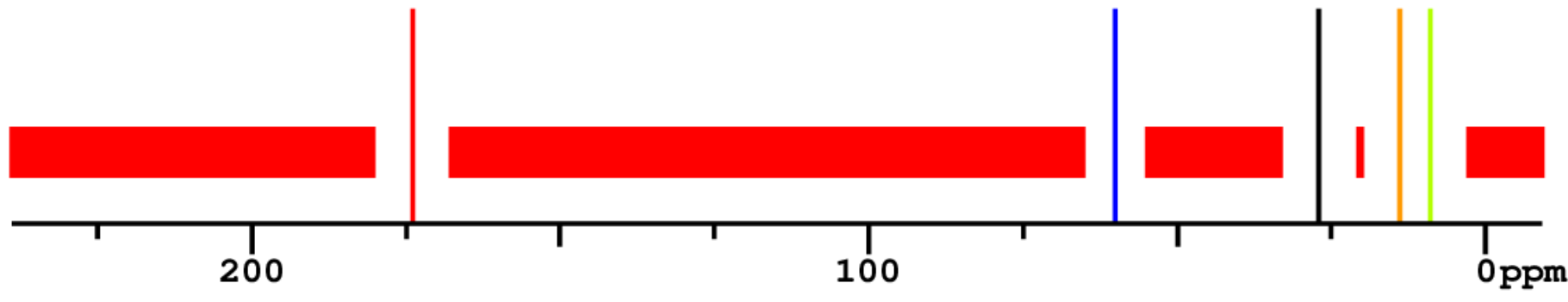
Structure Proposal #9

Structure	Similarity Measure
	<p>Deviation = 2.99 ppm Similarity = 100 %</p> <p>$C_6H_{14}O$</p> <p>MWT = 102.07</p> <p>Search Web for this structure: NUMQCACRALPSHD</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



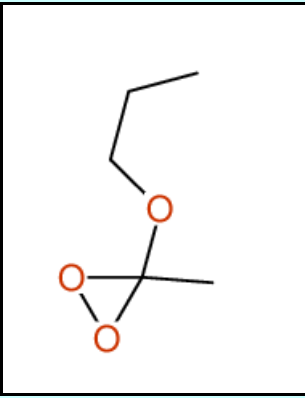
Experimental shift values

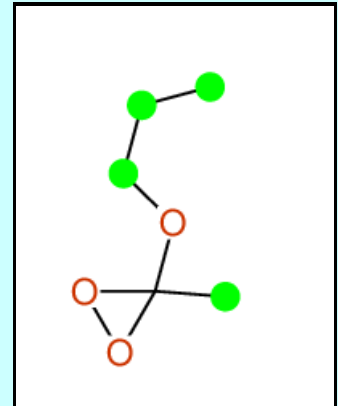
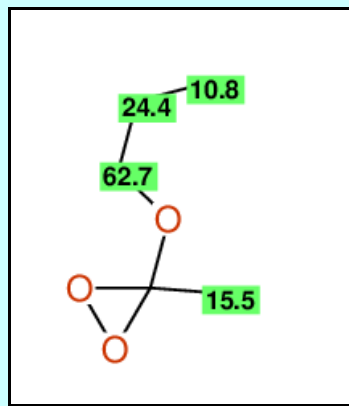
No line in reference: 



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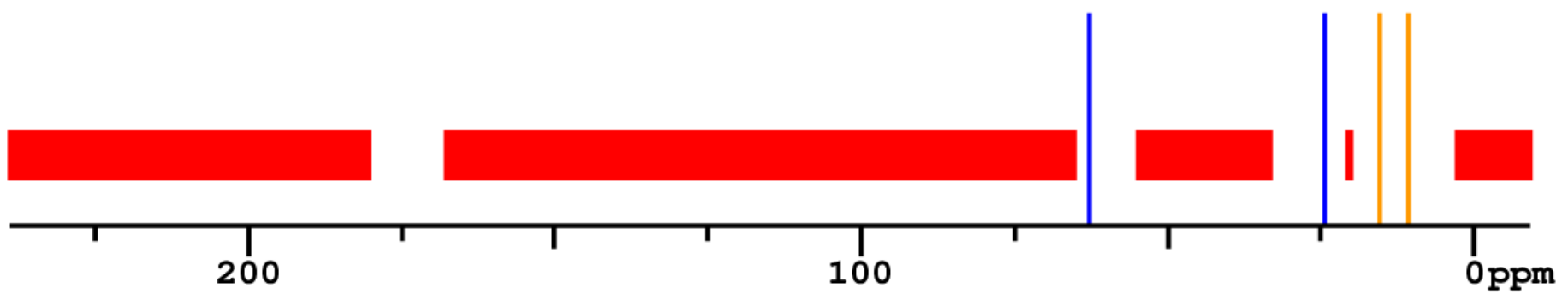
Structure Proposal #10

Structure	Similarity Measure
	<p>Deviation = 2.99 ppm Similarity = 100 %</p> <p>$C_5H_{10}O_3$</p> <p>MWT = 118.06</p> <p>Search Web for this structure: BZVVMENFRMWLO</p>
Predicted Chemical Shiftvalues	Matching Map



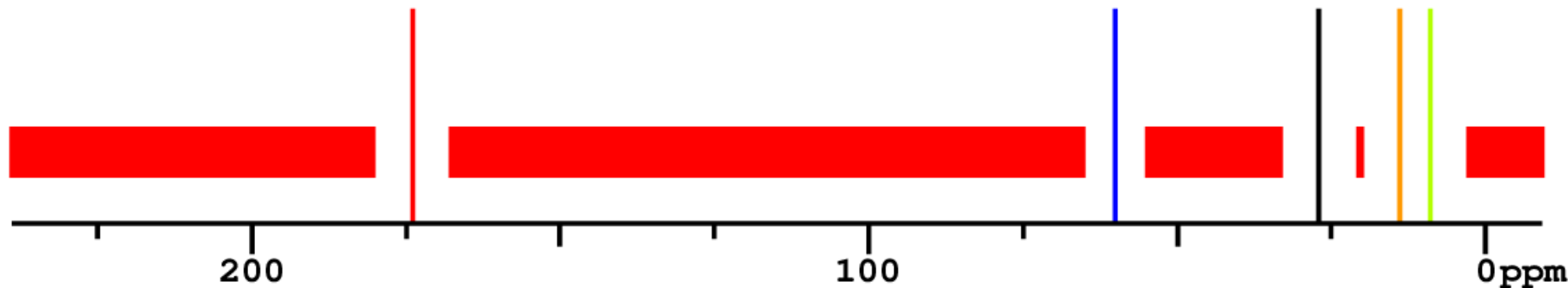
Predicted shift values

Signal multiplicity: S D T Q O E P ?



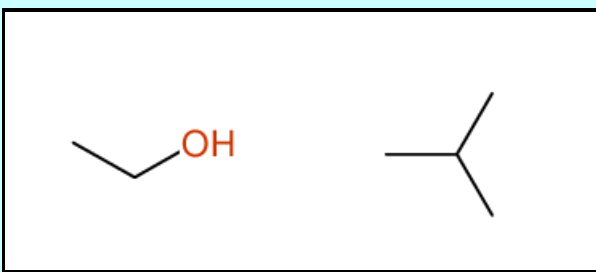

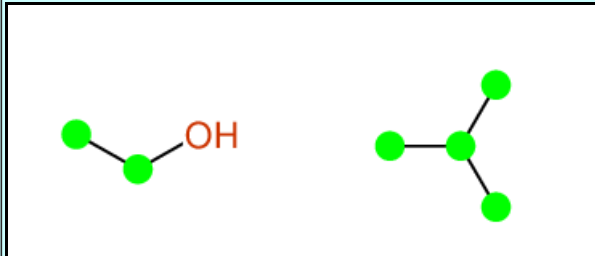
Experimental shift values

No line in reference: 



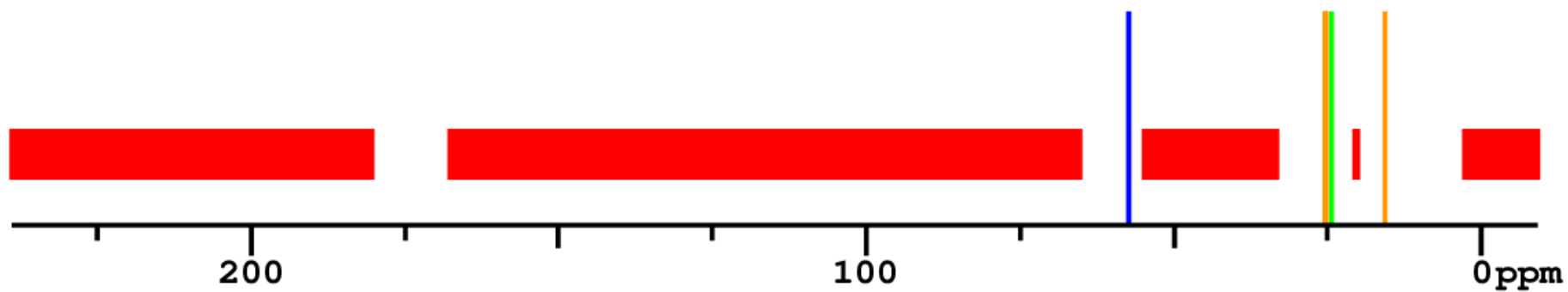
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Structure Proposal #11

Structure	Similarity Measure
	<p>Deviation = 3.07 ppm Similarity = 100 %</p> <p>$C_4H_{10} \cdot C_2H_6O$</p> <p>MWT = 104.07</p> <p>Search Web for this structure: GSKYFKHLAGYZDU</p>
Predicted Chemical Shiftvalues	Matching Map
	

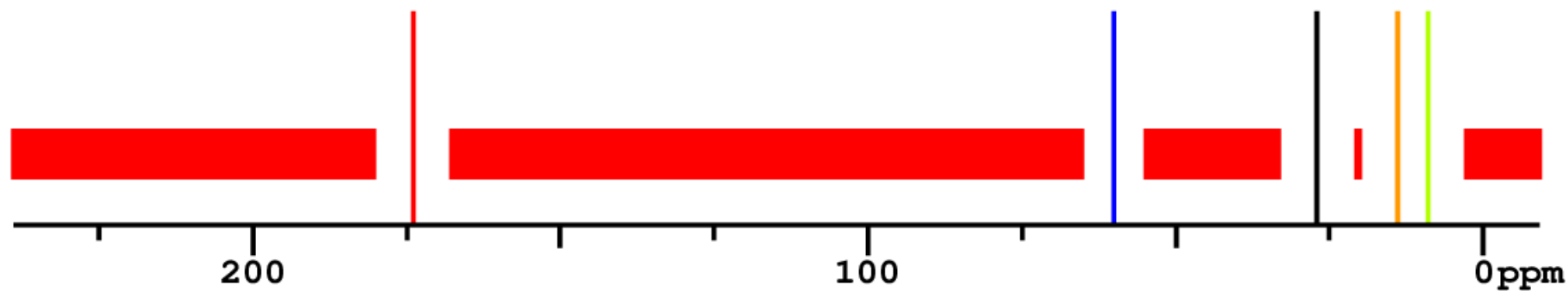
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

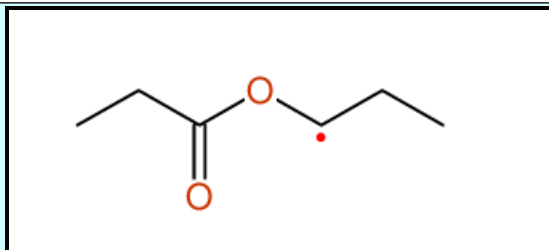
No line in reference: [red bar]



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Structure Proposal #12

Structure	Similarity Measure



Deviation = 3.24 ppm
 Similarity = 75 %
 (Different pattern)

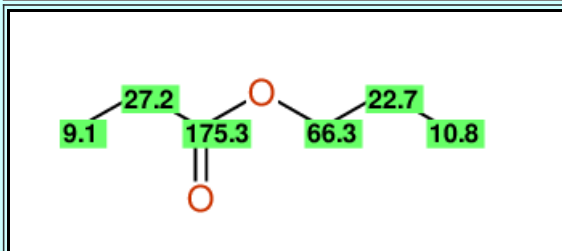
$C_6H_{11}O_2$

MWT = 115.07

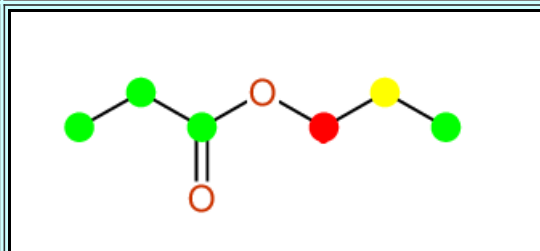
Search Web for this structure:

[CDQBJCILHGTWBX](#)

Predicted Chemical Shiftvalues

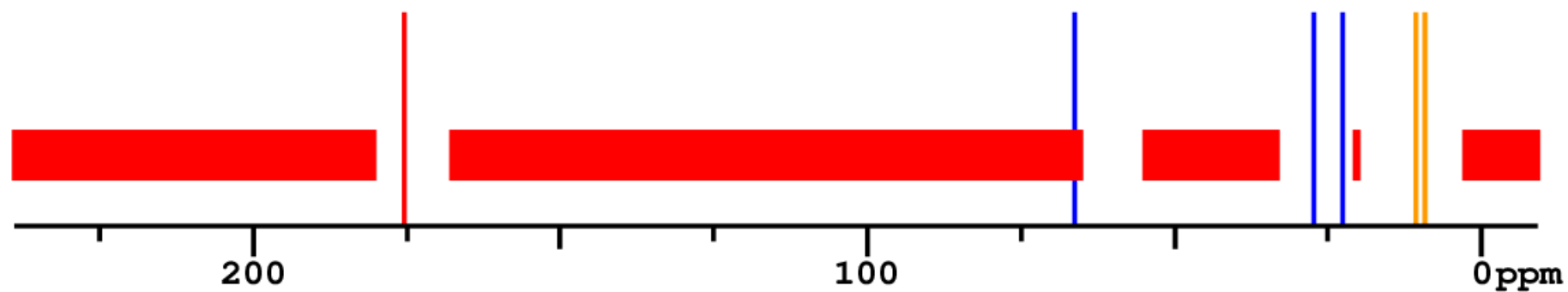


Matching Map




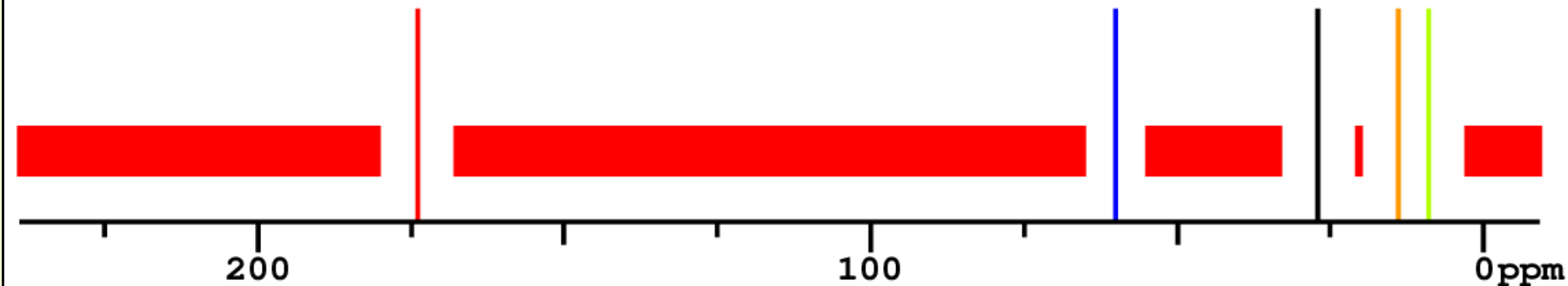
Predicted shift values

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



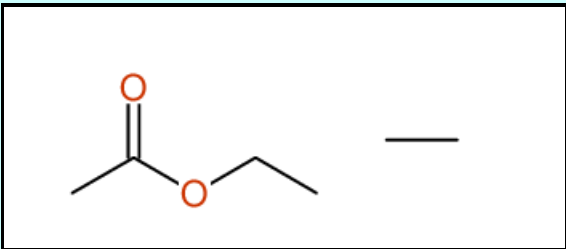
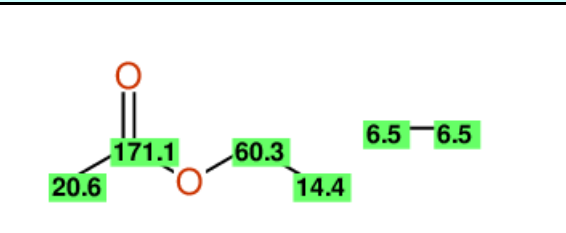
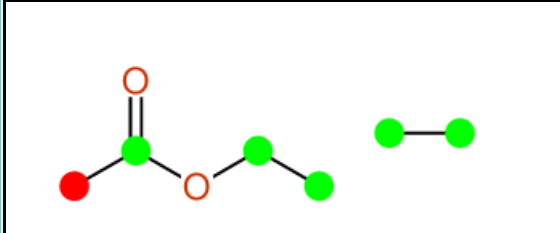
Experimental shift values

No line in reference: 



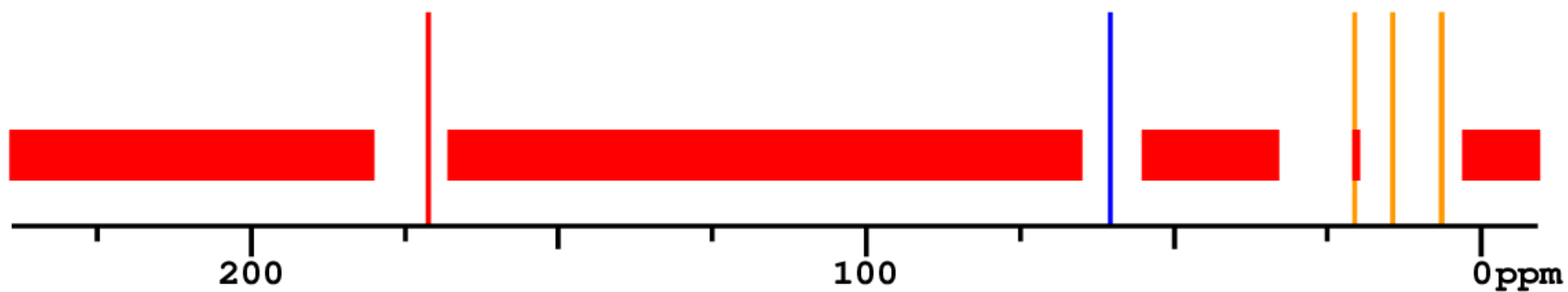
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Structure Proposal #13

Structure	Similarity Measure
	<p>Deviation = 3.27 ppm Similarity = 83 % (Different pattern)</p> <p>$C_4H_8O_2 \cdot C_2H_6$</p> <p>MWT = 118.07</p> <p>Search Web for this structure: ZRKANPPNISQQGA</p>
Predicted Chemical Shiftvalues	Matching Map
	

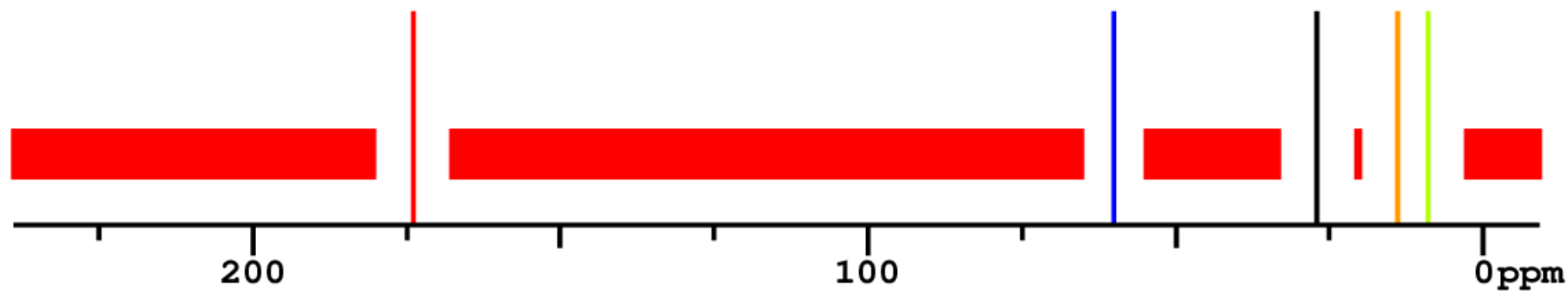
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

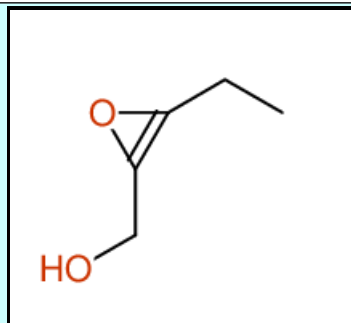
No line in reference: [red bar]



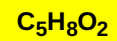
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Structure Proposal #14

Structure	Similarity Measure



Deviation = 3.32 ppm
Similarity = 100 %

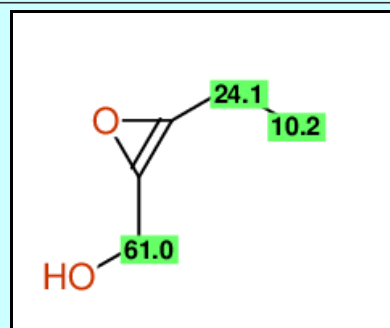


MWT = 100.06

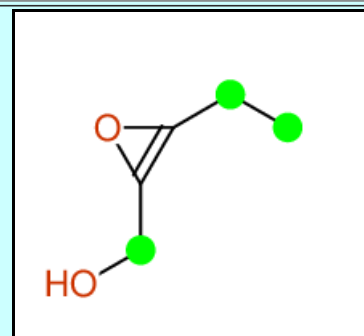
Search Web for this structure:

[ZZJKPPUKODAOML](#)

Predicted Chemical Shiftvalues

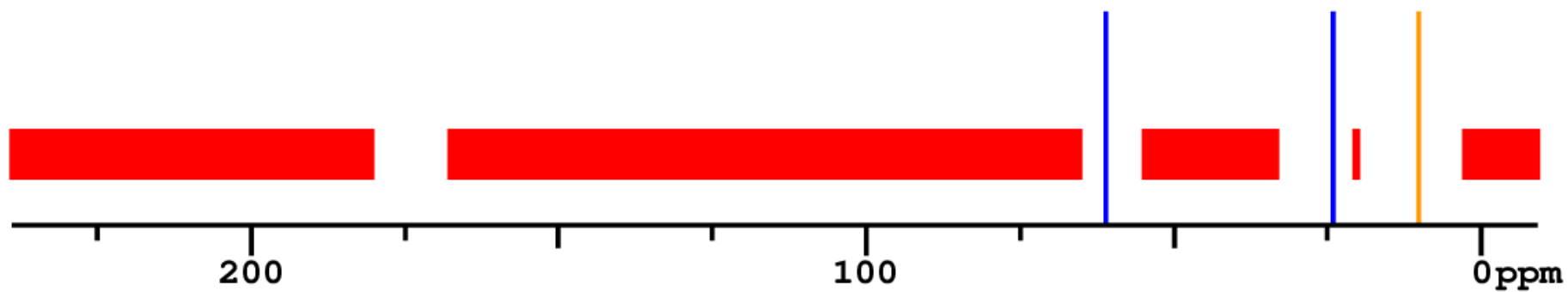


Matching Map



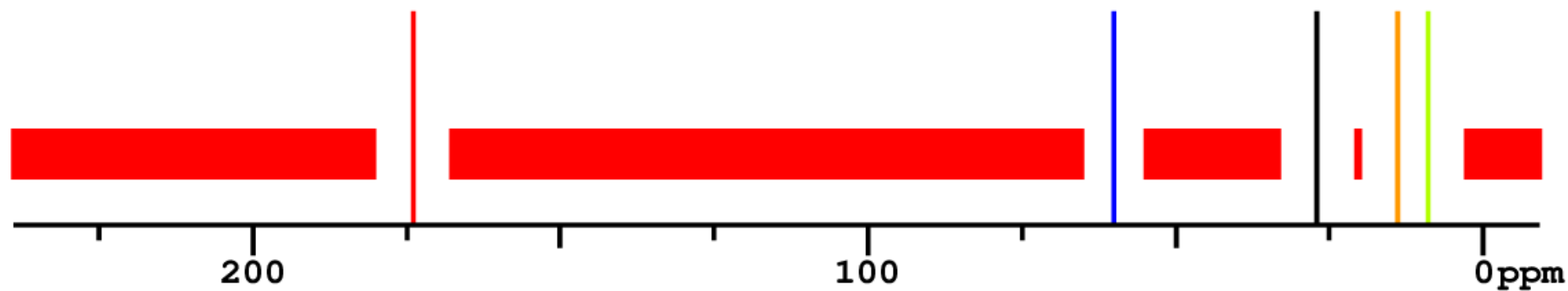
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

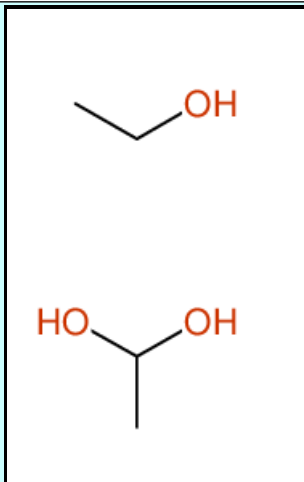
No line in reference: [red bar]



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Structure Proposal #15

Structure	Similarity Measure
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Deviation = 3.35 ppm
Similarity = 100 %

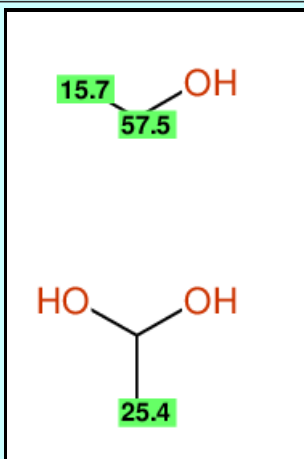
$\text{C}_2\text{H}_6\text{O}_2 \cdot \text{C}_2\text{H}_6\text{O}$

MWT = 108.04

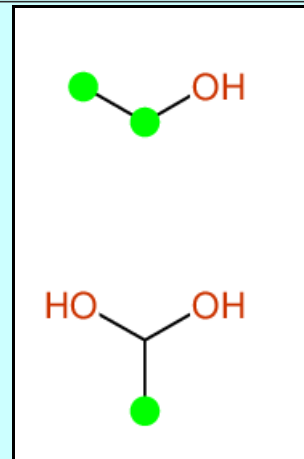
Search Web for this structure:

[WLPYHZGVXMAZET](#)

Predicted Chemical Shiftvalues

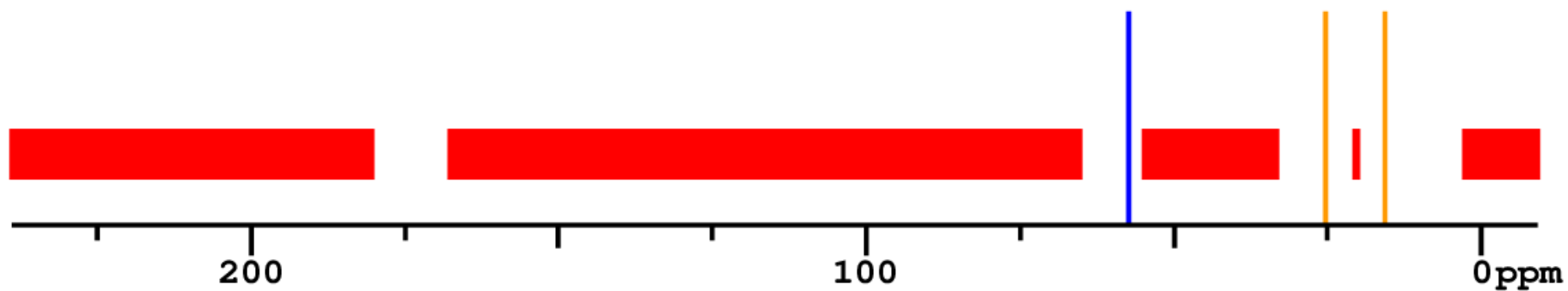


Matching Map



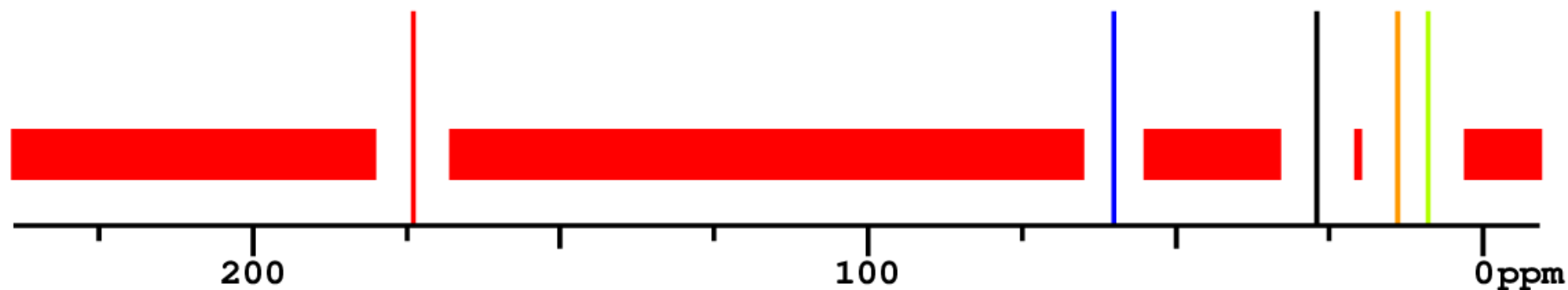
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

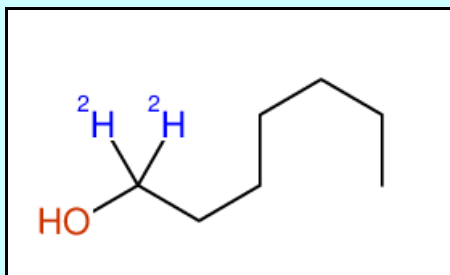
No line in reference: [red bar]



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Structure Proposal #16

Structure	Similarity Measure



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

$C_7H_{16}O$

MWT = 118.08

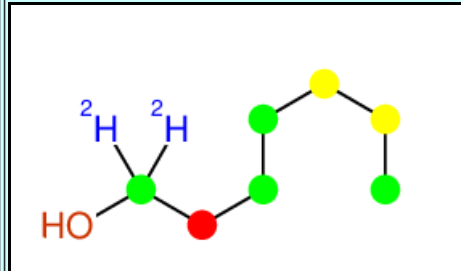
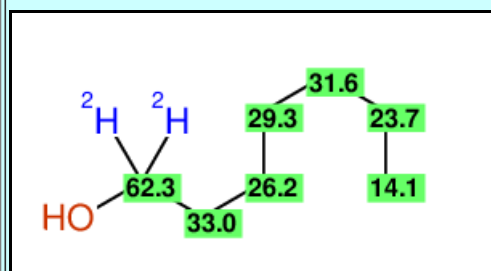
Search Web for this structure:

[BBMCTIGTTCKYKF](#)

[Availability](#)

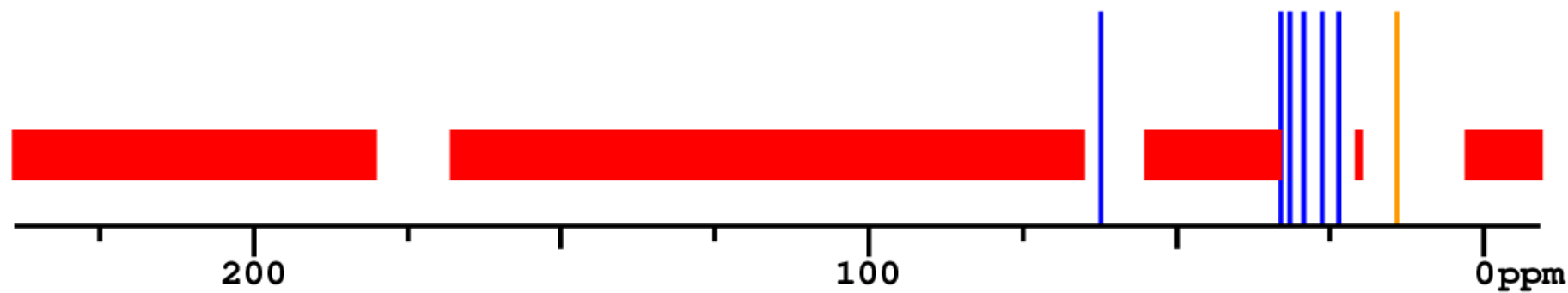
Predicted Chemical Shiftvalues

Matching Map



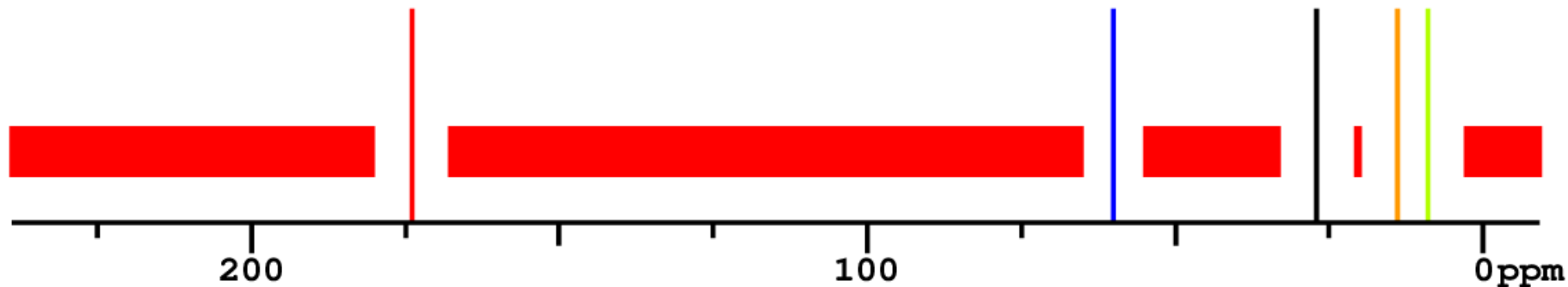
Predicted shift values

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



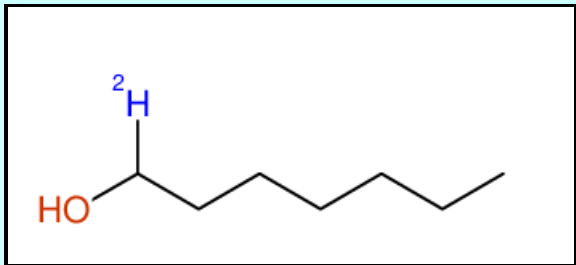
Experimental shift values

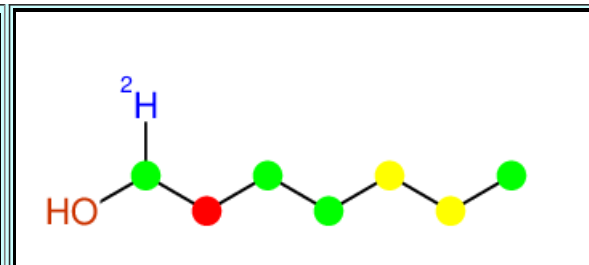
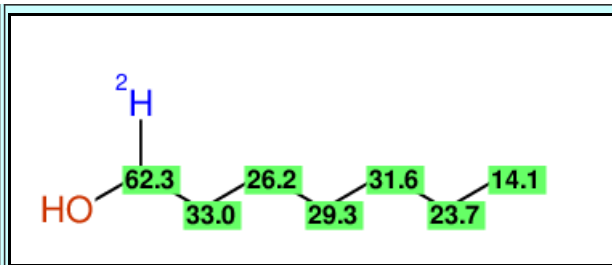
No line in reference:



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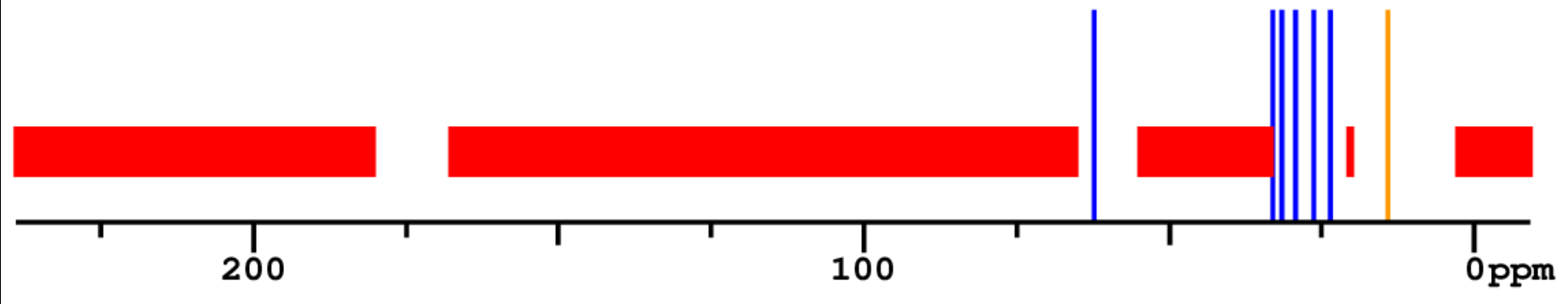
Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 3.38 ppm Similarity = 71 % (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 117.08</p> <p>Search Web for this structure: BBMCTIGTCKYKE</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



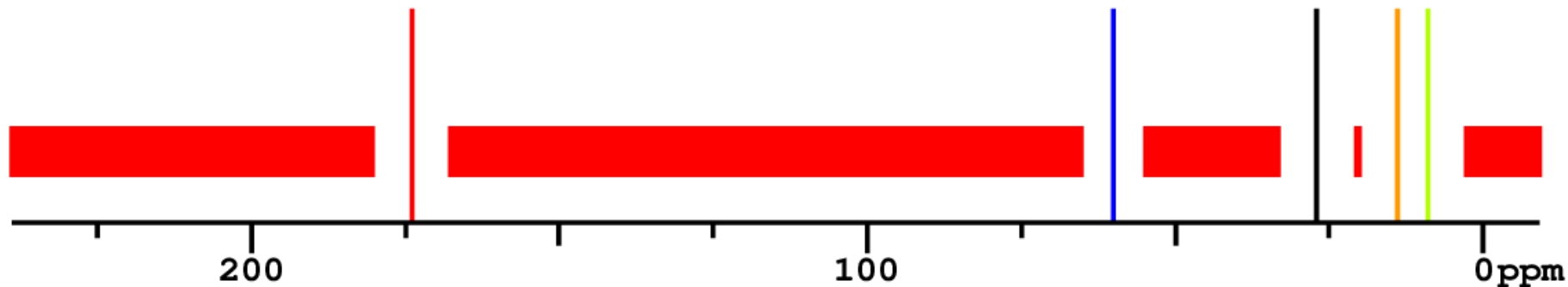
Predicted shift values

Signal multiplicity: S D T Q O E P ?



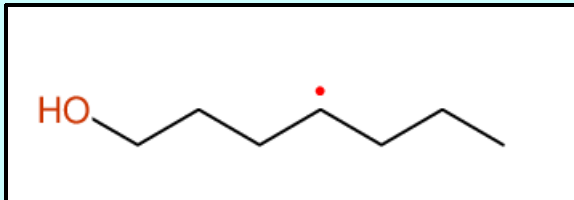
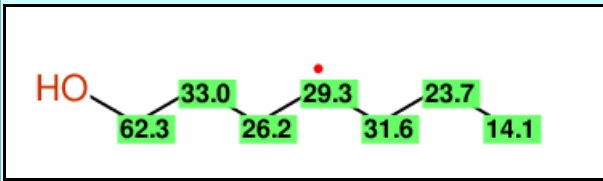

Experimental shift values

No line in reference: 



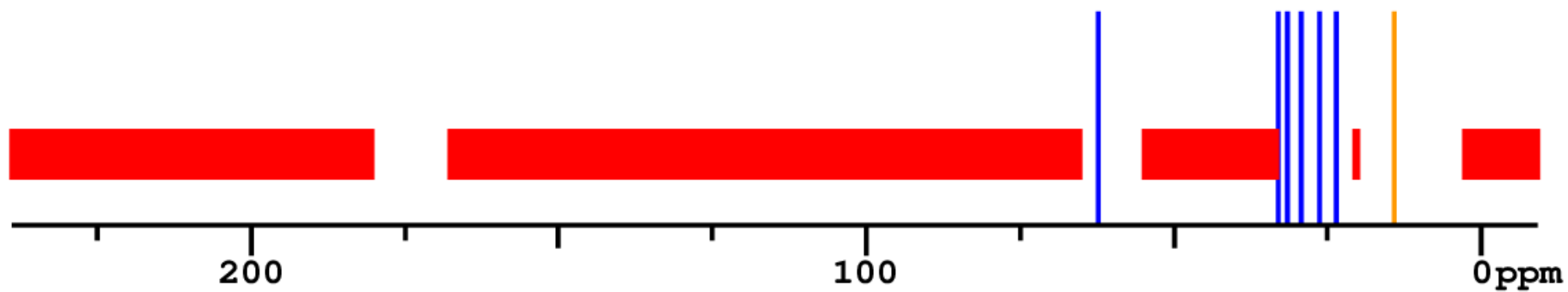
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Structure Proposal #18

Structure	Similarity Measure
	Deviation = 3.38 ppm Similarity = 71 % (Different pattern) $C_7H_{15}O$ MWT = 115.08 Search Web for this structure: GORPBXJSOXJRJC
Predicted Chemical Shiftvalues	Matching Map
	

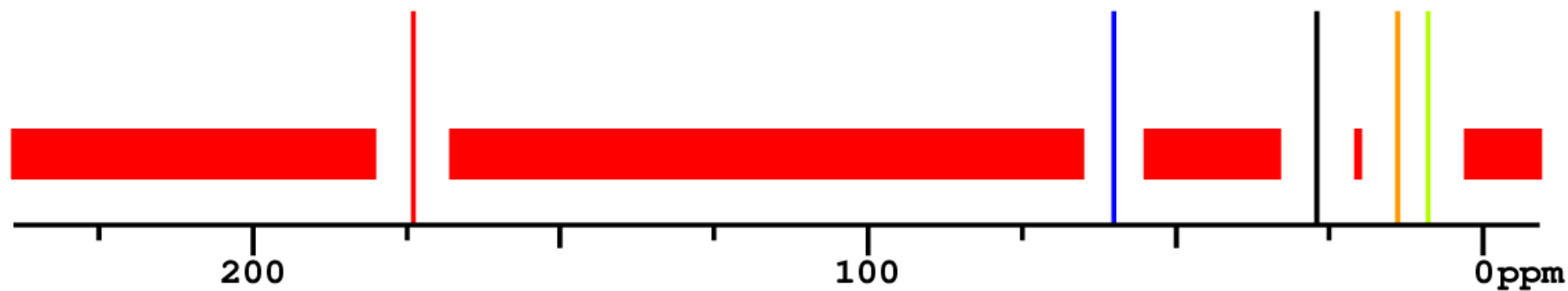
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

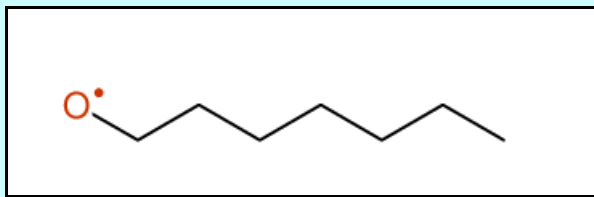
No line in reference: [red bar]



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Structure Proposal #19

Structure	Similarity Measure



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

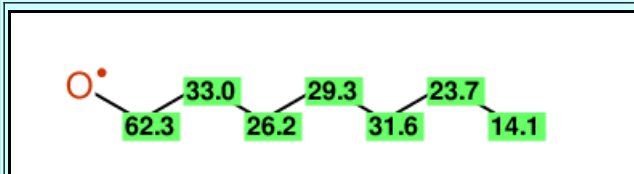
C₇H₁₅O

MWT = 115.08

Search Web for this structure:

[XBKKJRZFSVTKGZ](#)

Predicted Chemical Shiftvalues

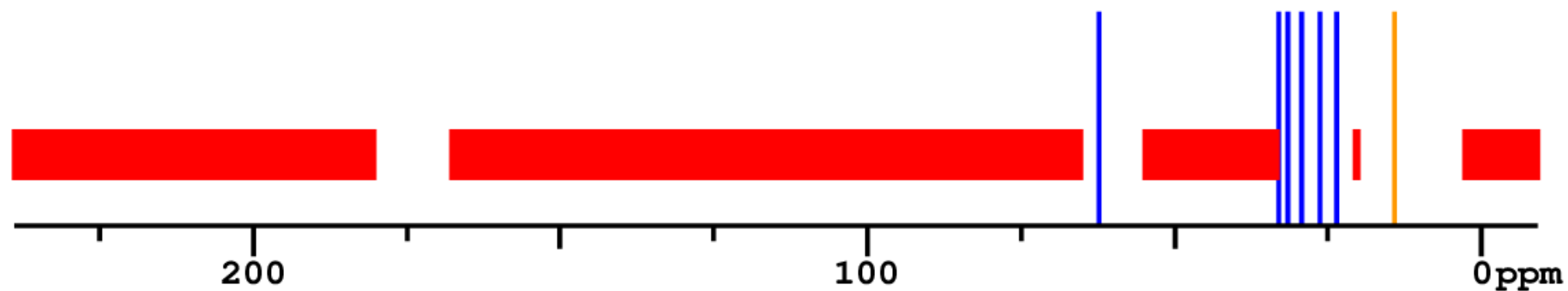


Matching Map




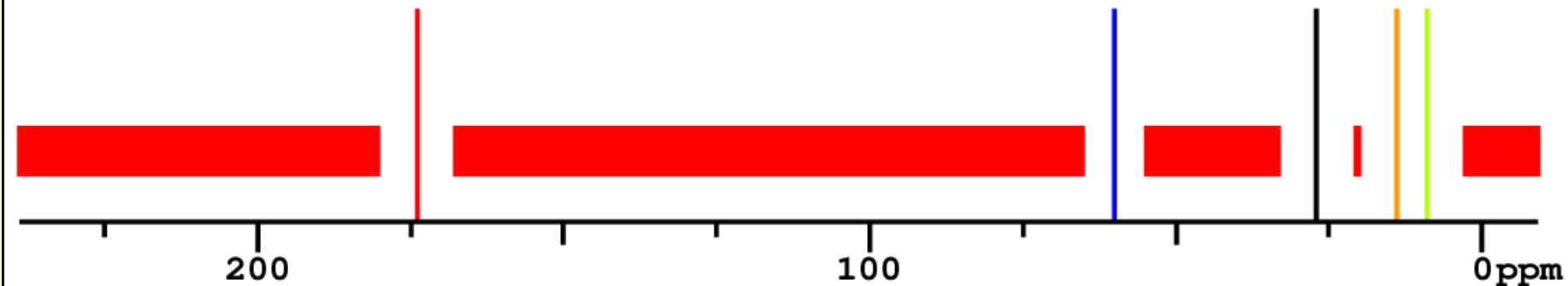
Predicted shift values

Signal multiplicity: S D T Q O E P ?



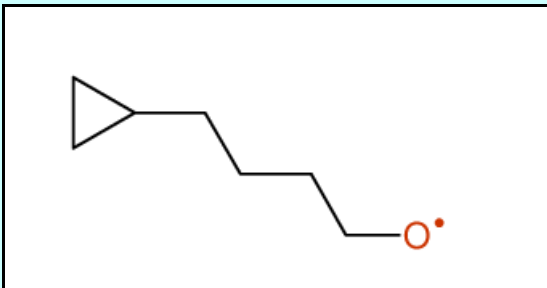
Experimental shift values

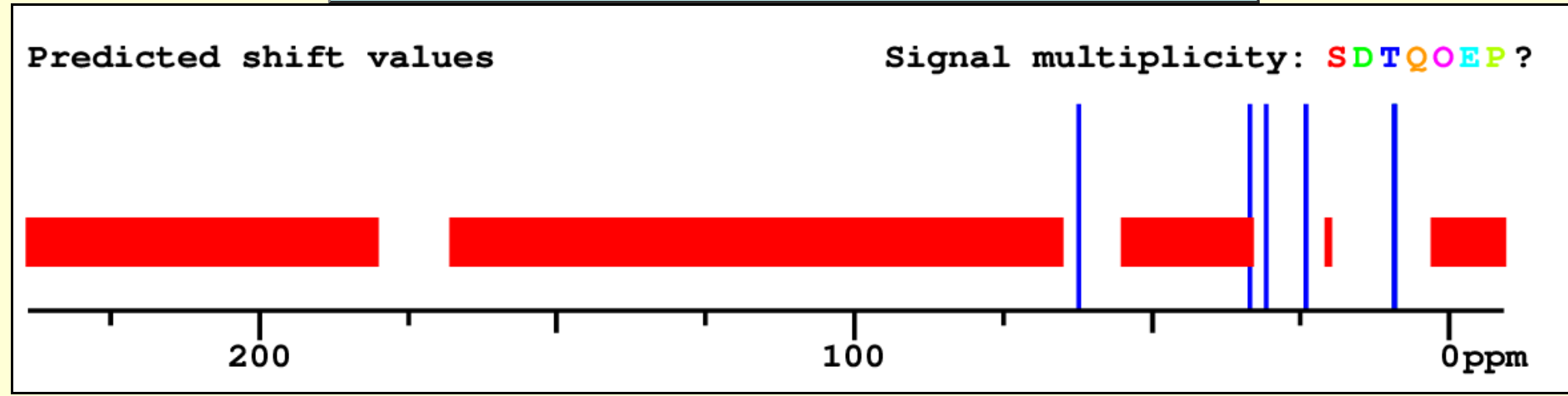
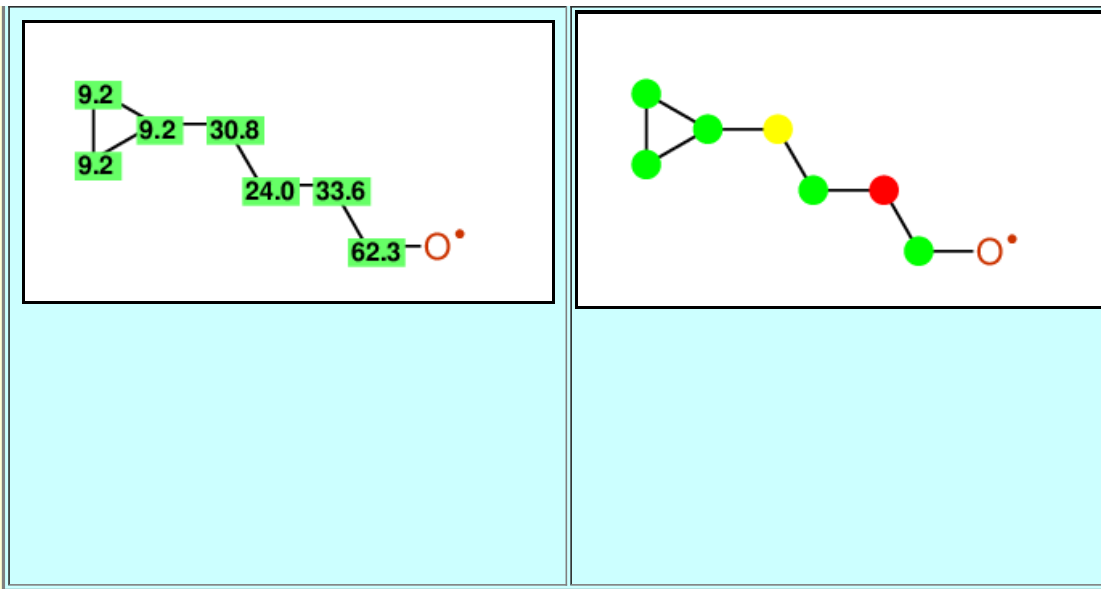
No line in reference: 



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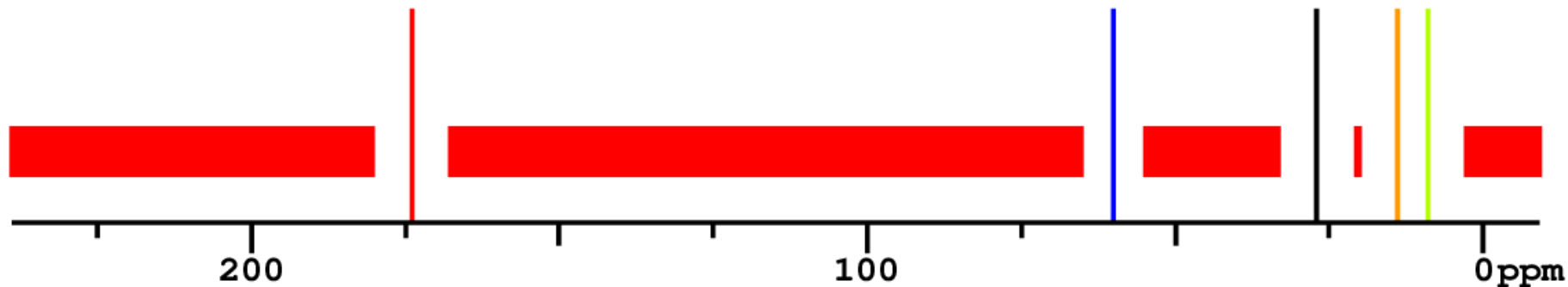
Structure Proposal #20

Structure	Similarity Measure
 <p>The chemical structure shows a cyclopropyl ring attached to a four-carbon chain. The terminal carbon of the chain is bonded to a red oxygen atom with a single bond and a red radical dot, representing a cyclopropylbutyl radical.</p>	<p>Deviation = 3.39 ppm Similarity = 79 % (Different pattern)</p> <p>$C_7H_{13}O$</p> <p>MWT = 113.08</p> <p>Search Web for this structure: FRESAHHZYKWMSE</p>
Predicted Chemical Shiftvalues	Matching Map



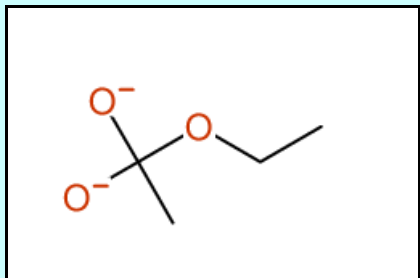
Experimental shift values

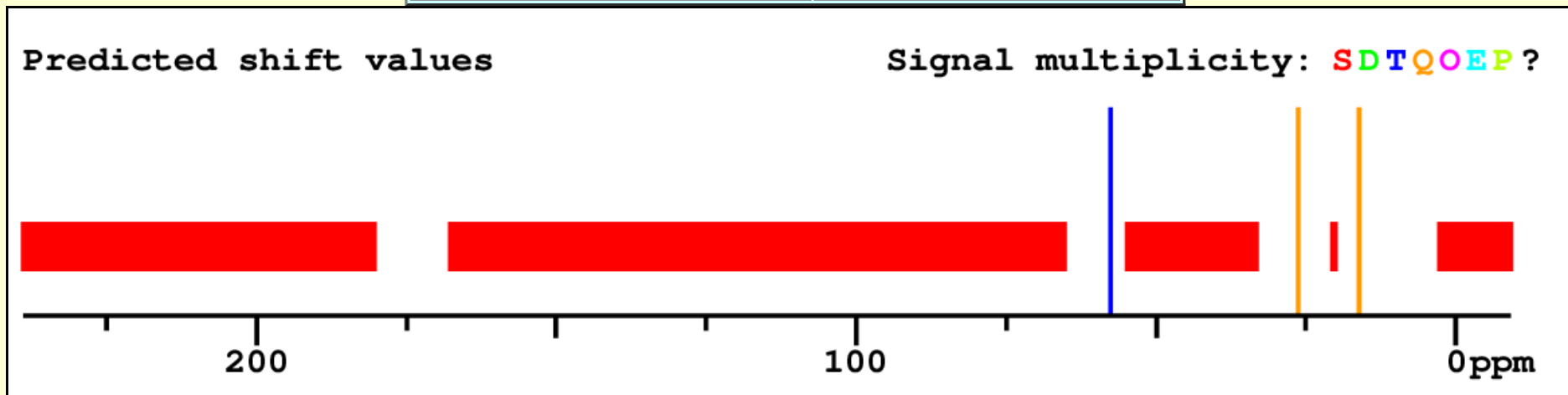
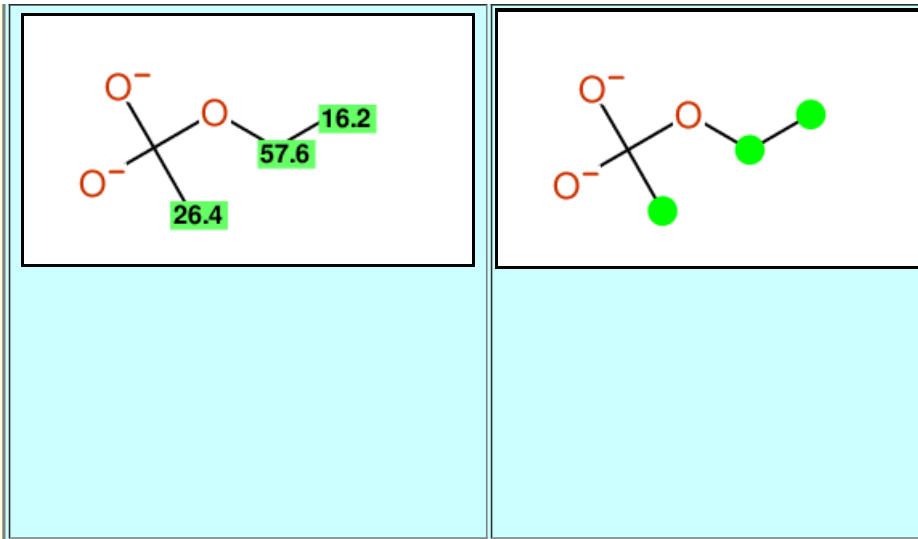
No line in reference: ████████



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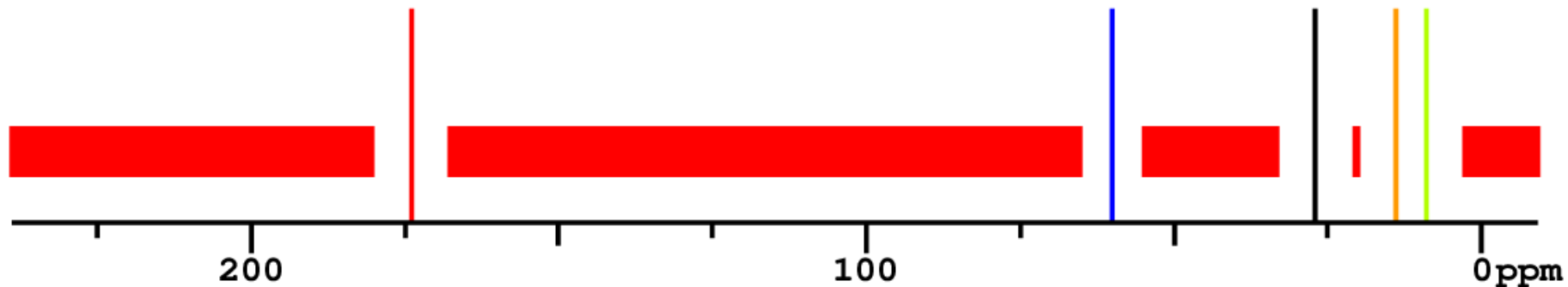
Structure Proposal #21

Structure	Similarity Measure
	Deviation = 3.40 ppm Similarity = 100 % $C_4H_8O_3$ MWT = 104.04 Search Web for this structure: QNBMMTAJSMBXKY
Predicted Chemical Shiftvalues	Matching Map



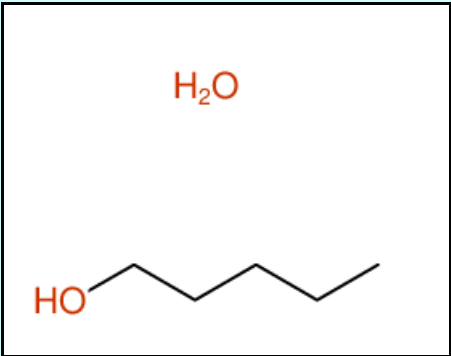
Experimental shift values

No line in reference: ████████



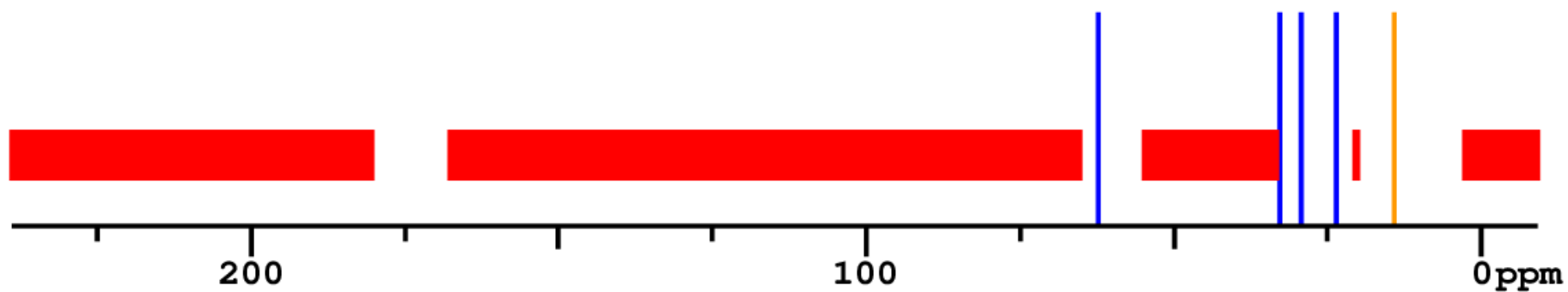
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Structure Proposal #22

Structure	Similarity Measure
	<p>Deviation = 3.40 ppm Similarity = 80 %</p> <p><chem>C5H12O.H2O</chem></p> <p>MWT = 106.06</p> <p>Search Web for this structure: LBFCRPJWCIHPSX</p>
Predicted Chemical Shiftvalues	Matching Map

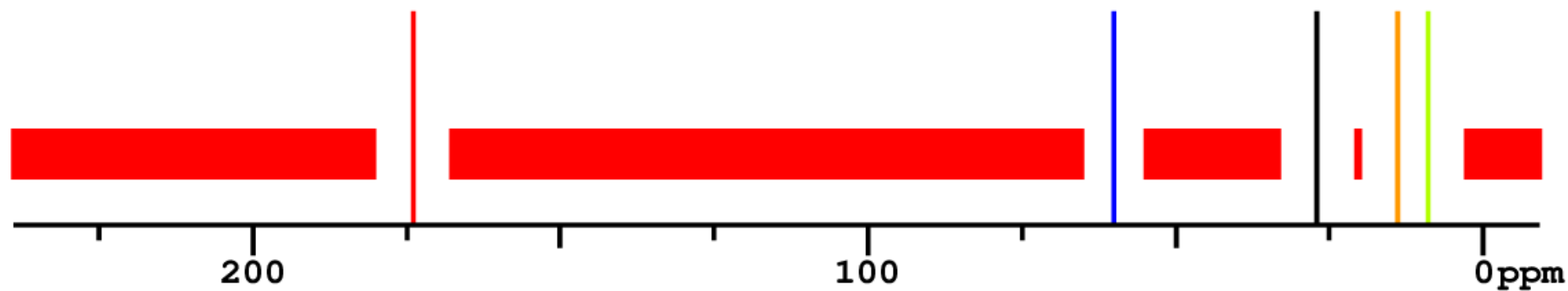
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

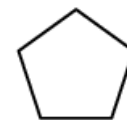


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Summary of the 2 most frequently occurring parent ring systems
within the 10 best-fitting entries

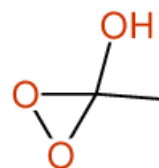
Occurrence:

1 in 10



Occurrence:

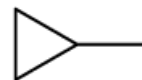
1 in 10



Summary of the 10 most frequently occurring parent ring systems
within the 152 best-fitting entries

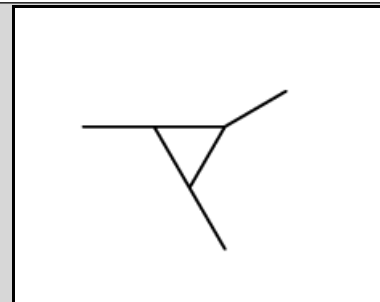
Occurrence:

9 in 152



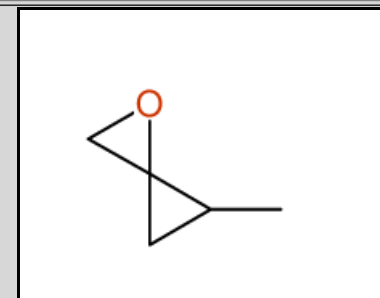
Occurrence:

7 in 152



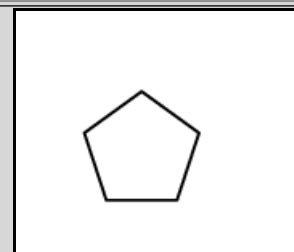
Occurrence:

2 in 152



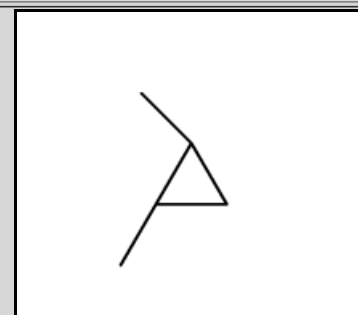
Occurrence:

1 in 152



Occurrence:

1 in 152



Occurence:

1 in 152



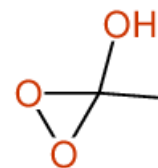
Occurence:

1 in 152



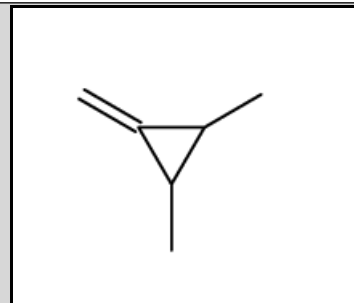
Occurence:

1 in 152



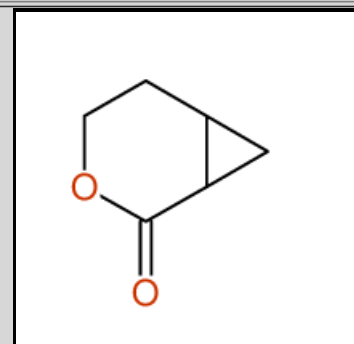
Occurrence:

1 in 152



Occurrence:

1 in 152



Summary of Processing

Checking existence of data and counting them:	177,099,966 entries in 3.174 seconds
Applying restraints from elemental composition:	8.921 seconds, 5,102,397 entries remain
Applying restraints from number of signals:	4.496 seconds, 218,318 entries remain
Searching 3,082,356,159 chemical shift values line-per-line:	29.825 seconds
Best 8,680 entries selected for analysis:	3.803 seconds
Ranking of 8,680 entries by similarity:	396.799 seconds
Deviation of best match:	0.81 ppm
Creating table and linking 8,680 structures to 475,803 INCHIKEY-pages:	0.981 seconds
Detailed Analysis of 23 structures including graphical representation:	7.943 seconds

Analysis of 152 structures for common parent ring systems:	0.018 seconds
Total CPU-usage:	457.830 seconds
Data transferred from disk:	1,785 MBytes out of 2,744,055 MBytes
Program version:	20200916_2-3D-zip/00
Machine:	I9-9900K / 16x3.60GHz
<p>Page written by Wolfgang Robien using CSEARCH-Technology Page written on 2021:05:19 at 19:08 Page finished on 2021:05:19 at 19:27</p> <p>Have a nice day !</p>	