

Spectral Similarity Search based on
107,426,223 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

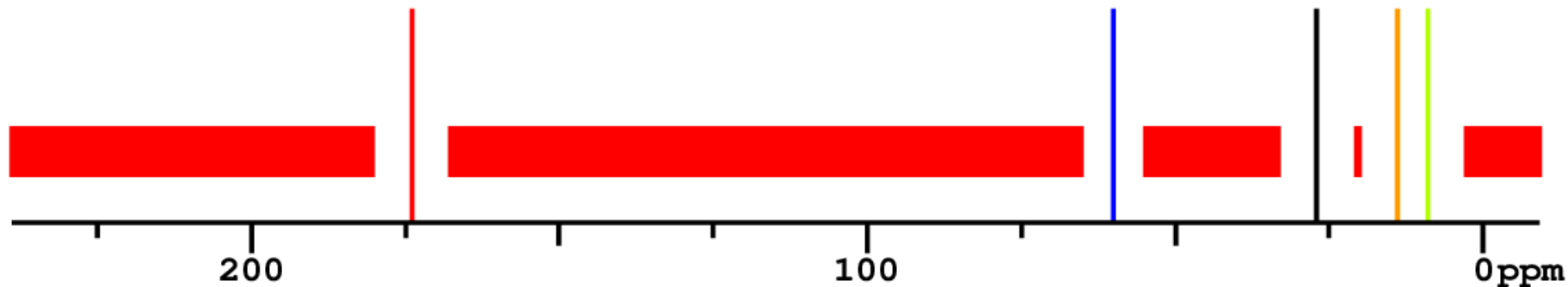
Name of Project:	Test1
Comment:	Dereplication-engine
Name of Compound:	Propionic_acid,ethylester 400MHz

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:	107,426,223
Compounds containing: N	100,077,635
Compounds containing: O	97,757,394
Compounds containing: P	827,023
Compounds containing: S	33,697,447
Compounds containing: F	20,533,163
Compounds containing: Cl	19,125,191
Compounds containing: Br	7,484,459
Compounds containing: I	1,114,581
Compounds containing: other	1,362,837

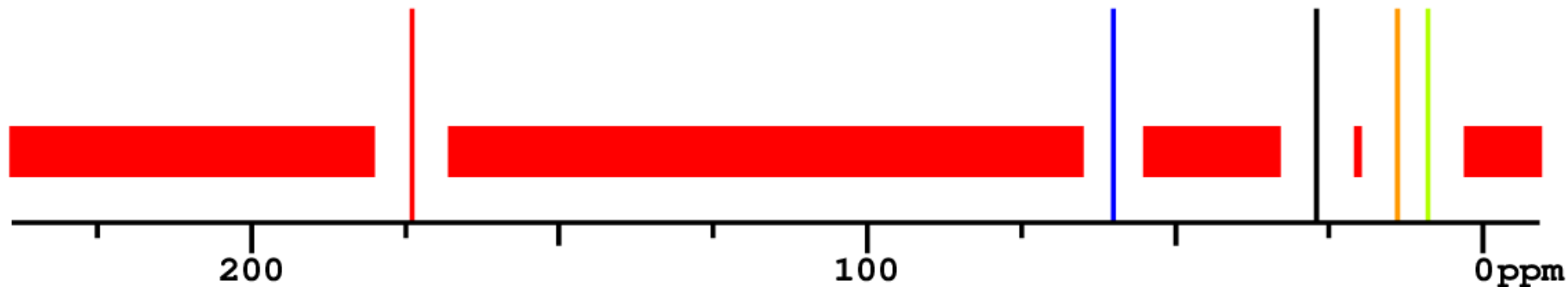
Available entries at each Screening-Step	
Total number of entries:	107,426,223

Applying requested elemental composition:	3,176,524 entries remain
Applying requested number of signals:	222,114 entries remain

Entries per line found out of 222,114 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	S	3.00	32,531	Unspecific line
2	60.00	T	2.50	25,468	Unspecific line
3	27.00	?	3.00	84,656	Unspecific line
4	14.00	Q	3.00	44,188	Unspecific line
5	9.00	P	3.00	29,978	Unspecific line

Experimental shift values

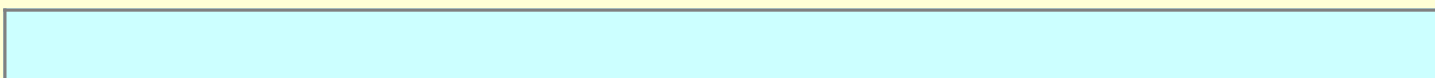
No line in reference: ██████████



Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	111	Selected for detailed analysis
4	1,417	Selected for detailed analysis
3	9,828	
2	42,160	
1	96,794	

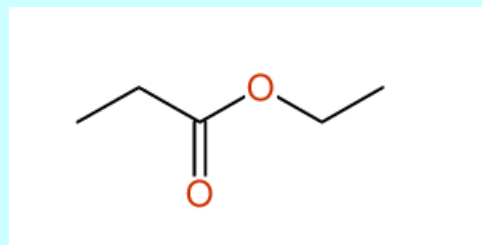
Best 17 Proposals shown for Compound: Propionic_acid,ethylester::400MHz



0.87 -
0.87ppm

3x found

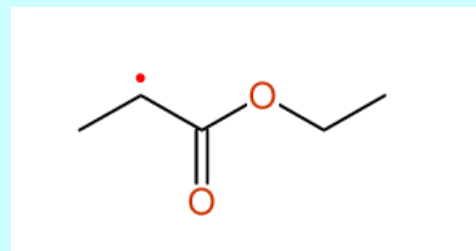
[FKRCODPIKNYEAC](#)



0.87 -
0.87ppm

1x found

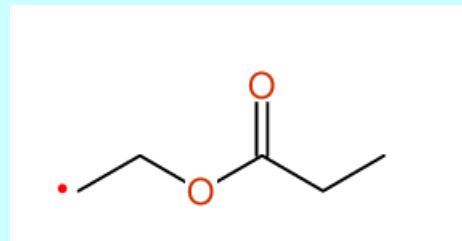
[UPLWNPAPKPCCE](#)



0.87 -
0.87ppm

1x found

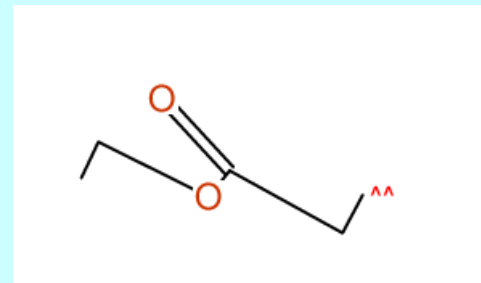
[IRGLFRDZYNBBCO](#)



0.87 -
0.87ppm

1x found

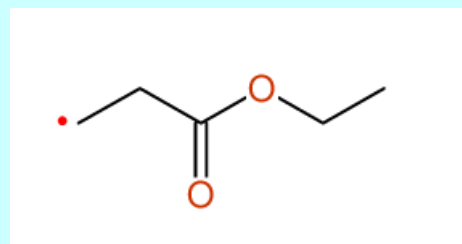
[BYLOWVUCDFUYIQ](#)



0.87 -
0.87ppm

1x found

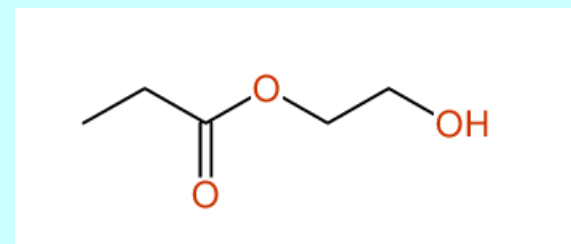
[SQKCNILPAQLIRC](#)



2.02 -
2.02ppm

1x found

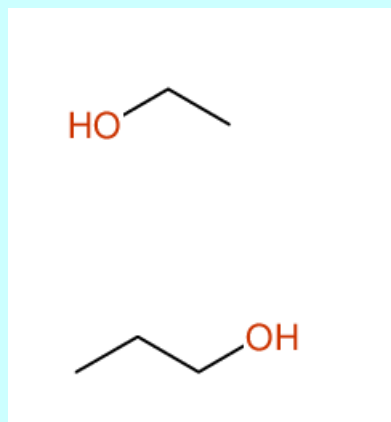
[SFAMKDPMPDEXGH](#)



2.62 -
2.62ppm

1x found

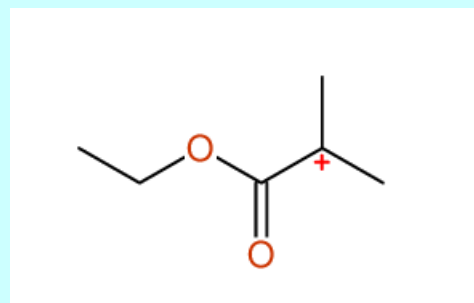
[OMRDZQXXMYCHBU](#)



2.93 -
2.93ppm

1x found

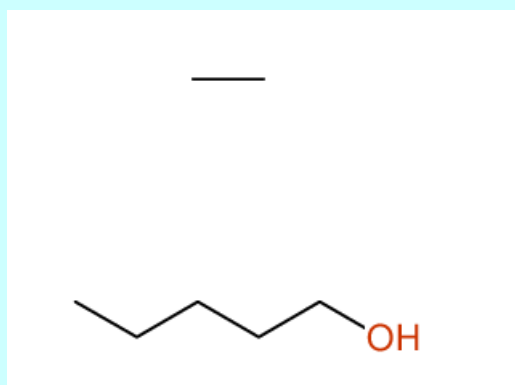
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2.98 -
2.98ppm

1x found

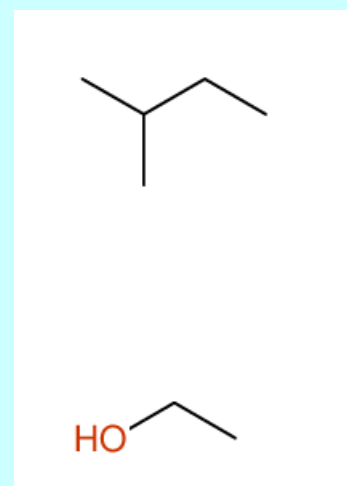
[ZARMDFHSJSIZKQ](#)



3.16 -
3.16ppm

1x found

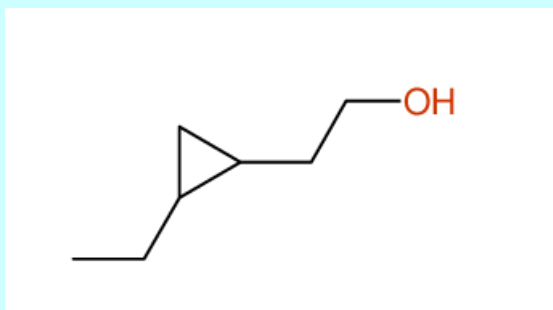
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3.49 -
3.49ppm

3x found

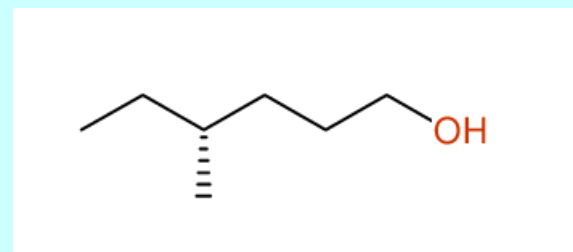
[IPKMDCPNAOYUEB](#)



4.01 -
4.01ppm

3x found

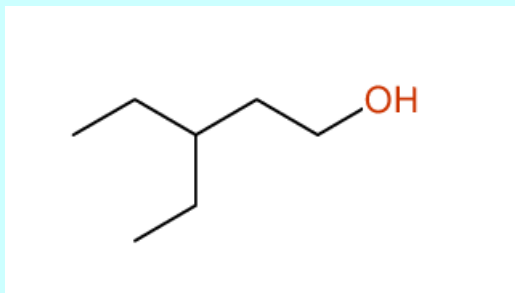
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4.36 -
4.36ppm

2x found

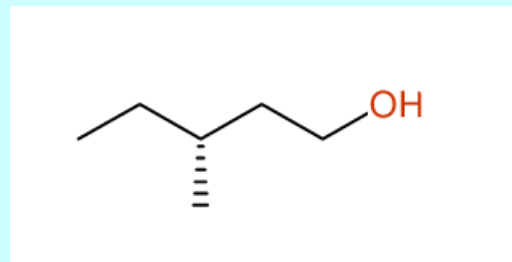
[DVEFUHVWJONKR](#)



4.64 -
4.64ppm

3x found

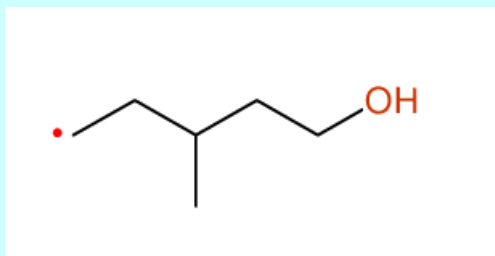
[IWTBVKIGCDZRPL](#)



4.64 -
4.64ppm

1x found

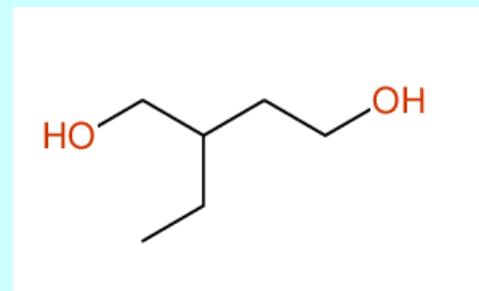
[FCACGIMTGMLTKJ](#)



4.98 -
4.98ppm

3x found

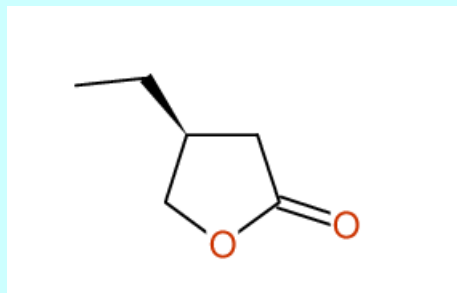
[CYVMBANVYOZFIG](#)



6.77 -
6.88ppm

3x found

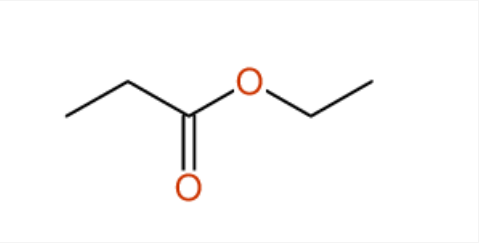

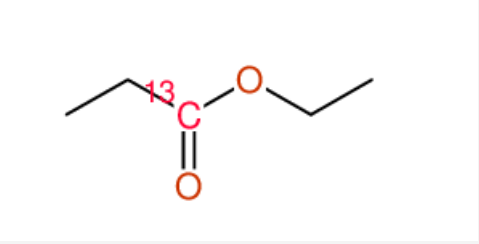

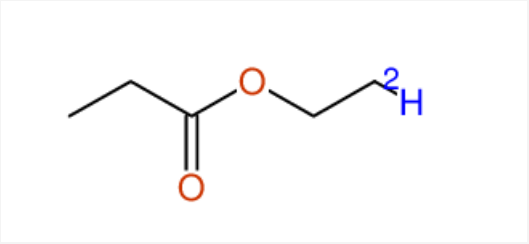

[MDQZVJSUBKPTHG](#)

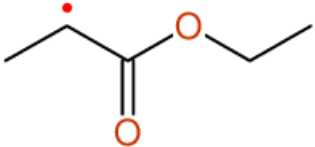
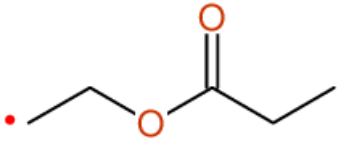
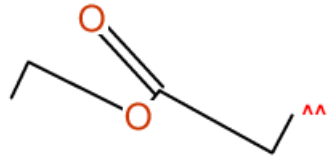
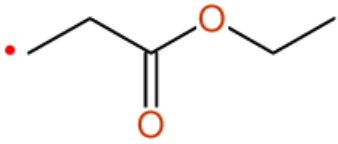


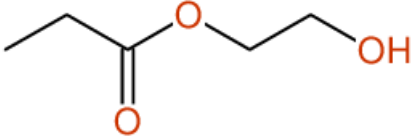
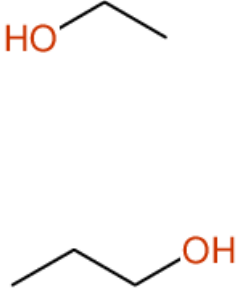
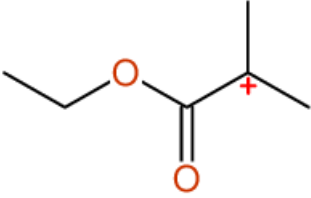
1,528 [Structure proposals](#) found for your C-NMR Spectrum

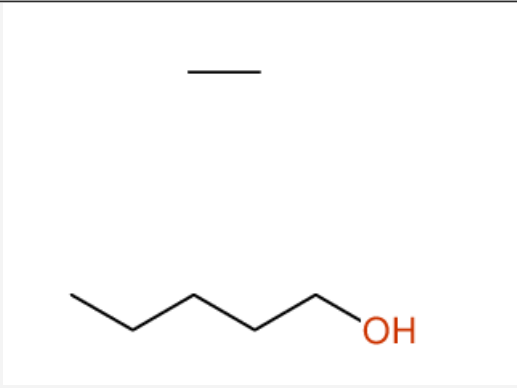
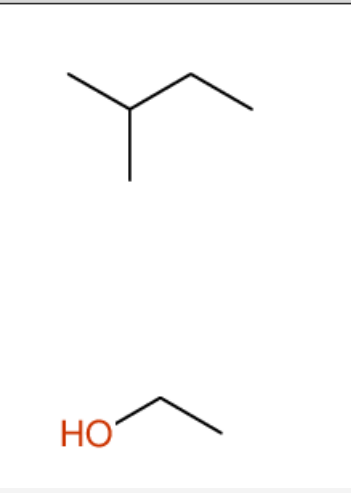
58 Entries will be shown because of your selection of additional constraints

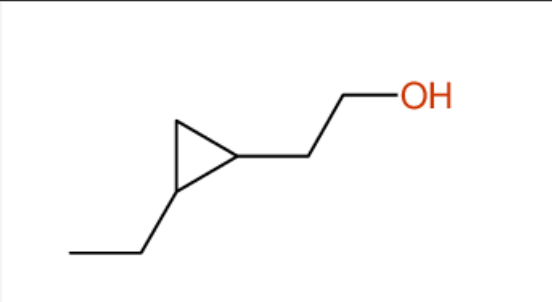

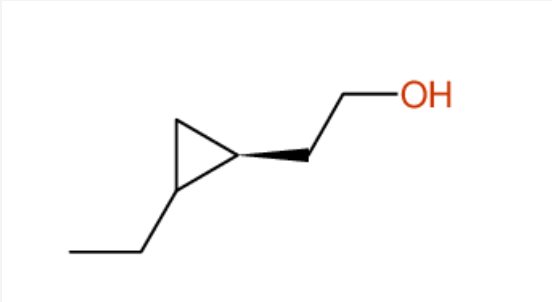

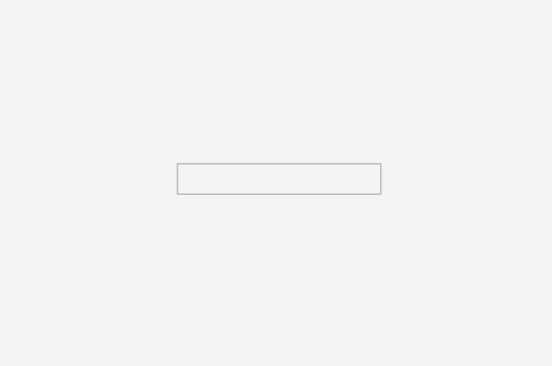

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼

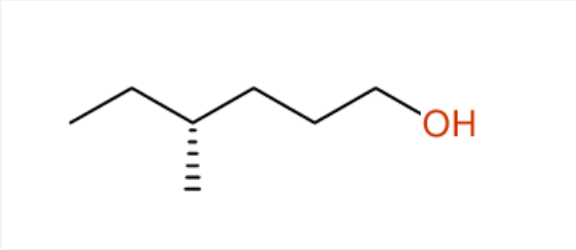

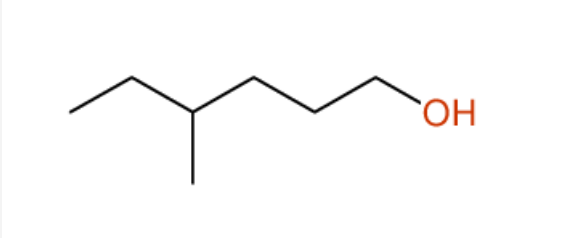

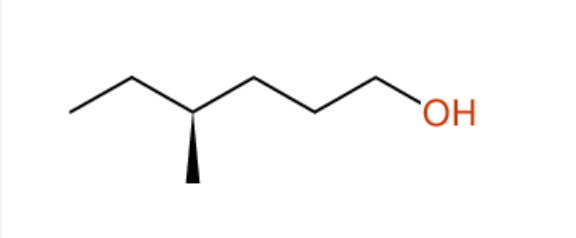

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #1</p> <p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 102.055</p>	<p>Proposal #1</p> <p>Structure-ID: 2,881,257</p> <p>FKRCODPIKNYEAC-UHFFFAOYAW</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #2</p> <p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 103.055</p>	<p>Proposal #2</p> <p>Structure-ID: 3,709,092</p> <p>FKRCODPIKNYEAC-HOSYLAQJED</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #3</p> <p>0.87</p> <p>Details</p>		<p>$C_5H_{10}O_2$</p> <p>MWT = 103.055</p>	<p>Proposal #3</p> <p>Structure-ID: 85,271,031</p> <p>FKRCODPIKNYEAC-VMNATFBREU</p>	<p>Availability of NMR-Data in CSEARCH</p> 

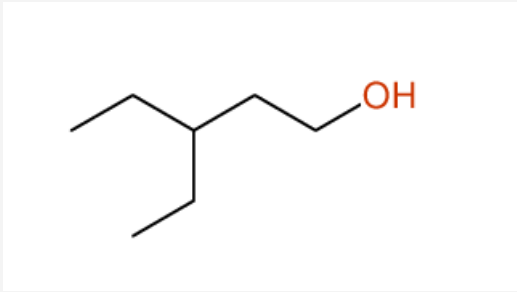

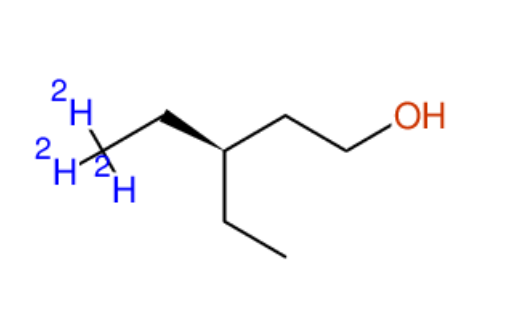

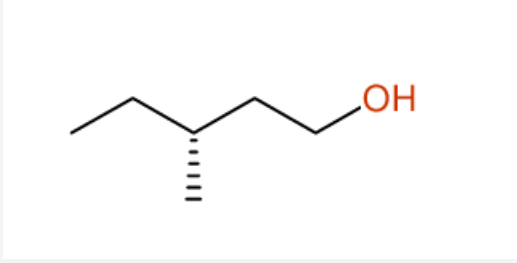

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #4 0.87 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #4 Structure-ID: 18,145,214 UPRLWNPAOPKPCE-UHFFFAOYAG	
Proposal #5 0.87 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #5 Structure-ID: 19,005,681 IRGLFRDZYNBBCO-UHFFFAOYAO	
Proposal #6 0.87 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #6 Structure-ID: 26,212,372 BYLOWVUCDFUYIQ-UHFFFAOYAU	
Proposal #7 0.87 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #7 Structure-ID: 3,764,581 SQKCNILPAQLIRC-UHFFFAOYAO	

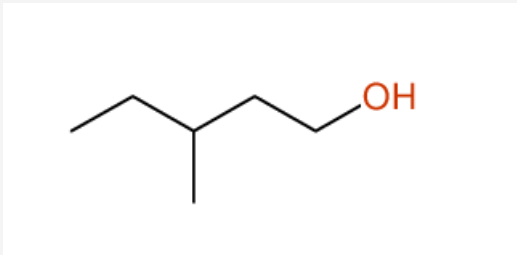

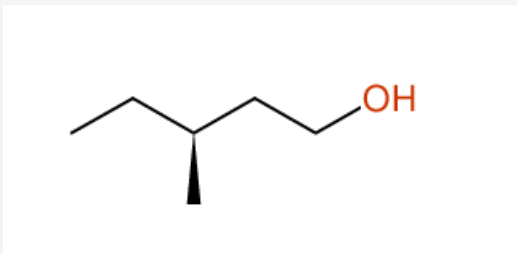

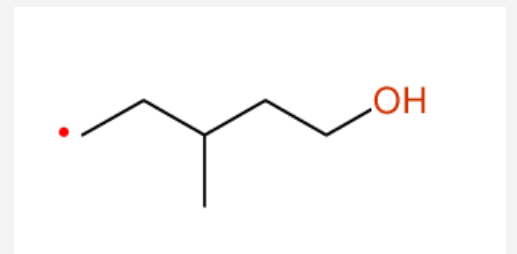
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #8</p> <p>2.02</p> <p>Details</p>		<p>$C_5H_{10}O_3$</p> <p>MWT = 118.055</p>	<p>Proposal #8</p> <p>Structure-ID: 4,551,455</p> <p>SFAMKDPMPDEXGH-UHFFFAOYAK</p>	
<p>Proposal #9</p> <p>2.62</p> <p>Details</p>		<p>$C_3H_8O.C_2H_6O$</p> <p>MWT = 106.055</p>	<p>Proposal #9</p> <p>Structure-ID: 21,914,558</p> <p>OMRDZQXXMYCHBU-UHFFFAOYAI</p>	
<p>Proposal #10</p> <p>2.93</p> <p>Details</p>		<p>$C_6H_{11}O_2$</p> <p>MWT = 115.066</p>	<p>Proposal #10</p> <p>Structure-ID: 102,709,334</p> <p>BNJCQKCNZHKCSF-UHFFFAOYAU</p>	

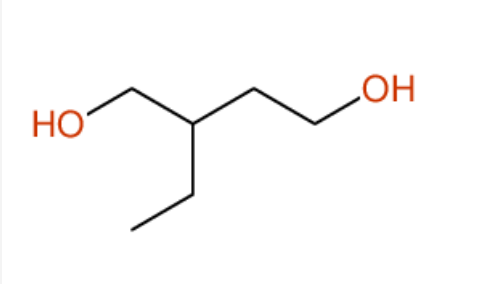
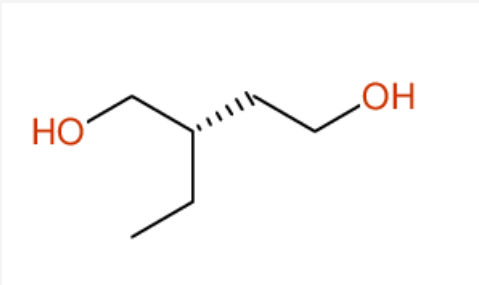
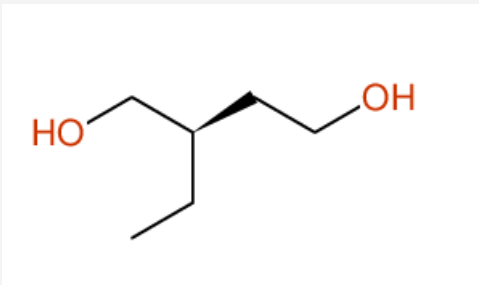
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #11</p> <p>2.98</p> <p>Details</p>		<p>$C_5H_{12}O \cdot C_2H_6$</p> <p>MWT = 118.077</p>	<p>Proposal #11</p> <p>Structure-ID: 45,792,163</p> <p>ZARMDFHSJSIZKQ-UHFFFAOYAM</p>	
<p>Proposal #12</p> <p>3.16</p> <p>Details</p>		<p>$C_5H_{12} \cdot C_2H_6O$</p> <p>MWT = 118.077</p>	<p>Proposal #12</p> <p>Structure-ID: 28,984,115</p> <p>FOXQTCHXXJKLNK-UHFFFAOYAU</p>	

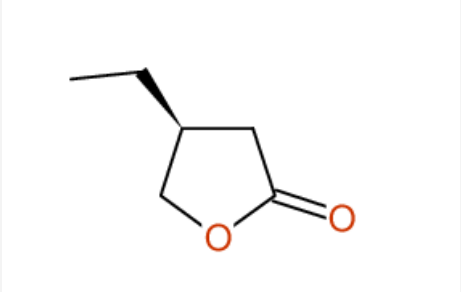

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #13 3.49 Details Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #13 Structure-ID: 29,976,720 IPKMDCPNAOYUEB-UHFFFAOYAW	Availability of NMR-Data in CSEARCH 
Proposal #14 3.49 Details Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #14 Structure-ID: 96,618,282 IPKMDCPNAOYUEB-COBESHVIPBN	Availability of NMR-Data in CSEARCH 
Proposal #15 3.49 Details Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #15 Structure-ID: 58,108,346 IPKMDCPNAOYUEB-RNFRBKRXBM	Availability of NMR-Data in CSEARCH 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #16</p> <p>4.01</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #16</p> <p>Structure-ID: 24,932,452</p> <p>YNPVNLWKVZZBTM-SSDOTTSWBB</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #17</p> <p>4.01</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #17</p> <p>Structure-ID: 2,959,629</p> <p>YNPVNLWKVZZBTM-UHFFFAOYAR</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #18</p> <p>4.01</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{16}O$</p> <p>MWT = 116.077</p>	<p>Proposal #18</p> <p>Structure-ID: 24,932,451</p> <p>YNPVNLWKVZZBTM-ZETCQYMHBD</p>	<p>Availability of NMR-Data in CSEARCH</p> 

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #19 4.36 Details Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #19 Structure-ID: 4,632,733 DVEFUHVWVWJONKR-UHFFFAOYAO	Availability of NMR-Data in CSEARCH 
Proposal #20 4.36 Details Different pattern		$C_7H_{16}O$ MWT = 119.077	Proposal #20 Structure-ID: 5,628,606 DVEFUHVWVWJONKR-AQNNMFFJFI	Availability of NMR-Data in CSEARCH 
Proposal #21 4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #21 Structure-ID: 19,143,410 IWTBVKIGCDZRPL-ZCFIWIBFBO	Availability of NMR-Data in CSEARCH 

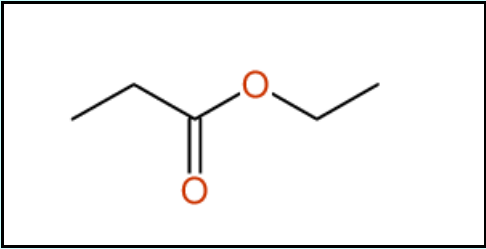
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #22 4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #22 Structure-ID: 2,884,586 IWTBVKIGCDZRPL-UHFFFAOYAP	Availability of NMR-Data in CSEARCH 
Proposal #23 4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #23 Structure-ID: 4,632,731 IWTBVKIGCDZRPL-LURJTMIEBM	Availability of NMR-Data in CSEARCH 
Proposal #24 4.64 Details Different pattern		$C_6H_{13}O$ MWT = 101.066	Proposal #24 Structure-ID: 50,404,314 FCACGIMTGMLTKJ-UHFFFAOYAW	

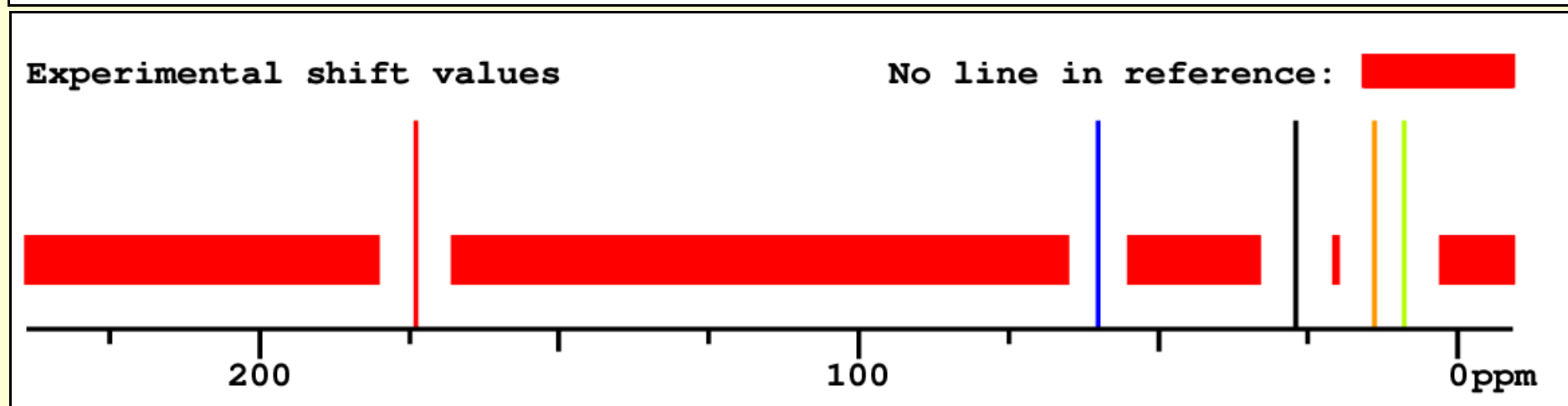
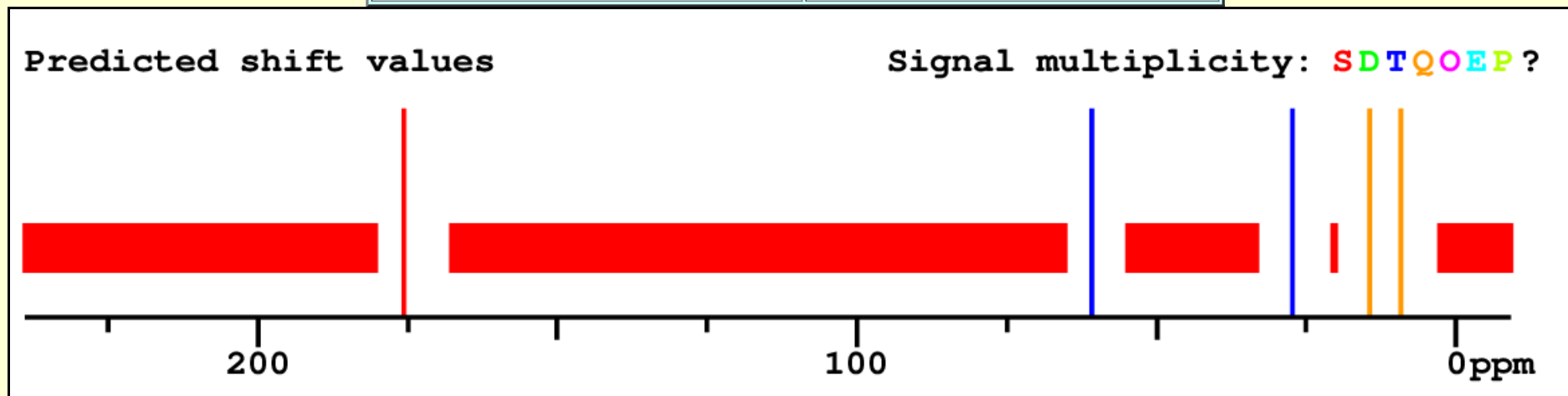
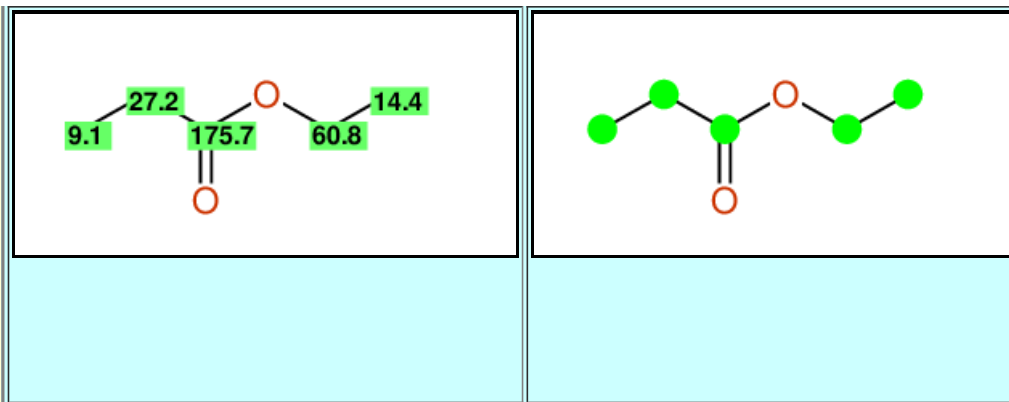
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #25</p> <p>4.98</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #25</p> <p>Structure-ID: 3,779,157</p> <p>CYVMBANVYOZFIG-UHFFFAOYAB</p>	
<p>Proposal #26</p> <p>4.98</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #26</p> <p>Structure-ID: 3,779,158</p> <p>CYVMBANVYOZFIG-LURJTMIEBY</p>	
<p>Proposal #27</p> <p>4.98</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{14}O_2$</p> <p>MWT = 118.066</p>	<p>Proposal #27</p> <p>Structure-ID: 3,480,926</p> <p>CYVMBANVYOZFIG-ZCFIWIBFBA</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #28 6.77 Details Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #28 Structure-ID: 51,765,446 MDQZVJSUBKPTHG-YFKPBYRVBH	Availability of NMR-Data in CSEARCH 

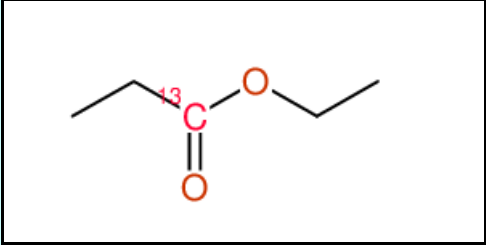
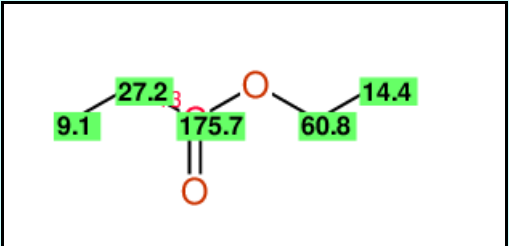
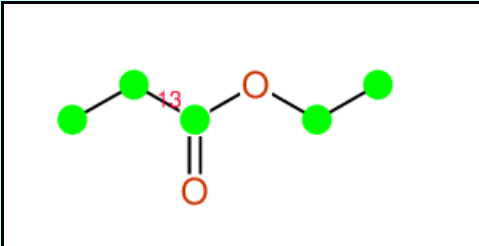
Detailed Analysis

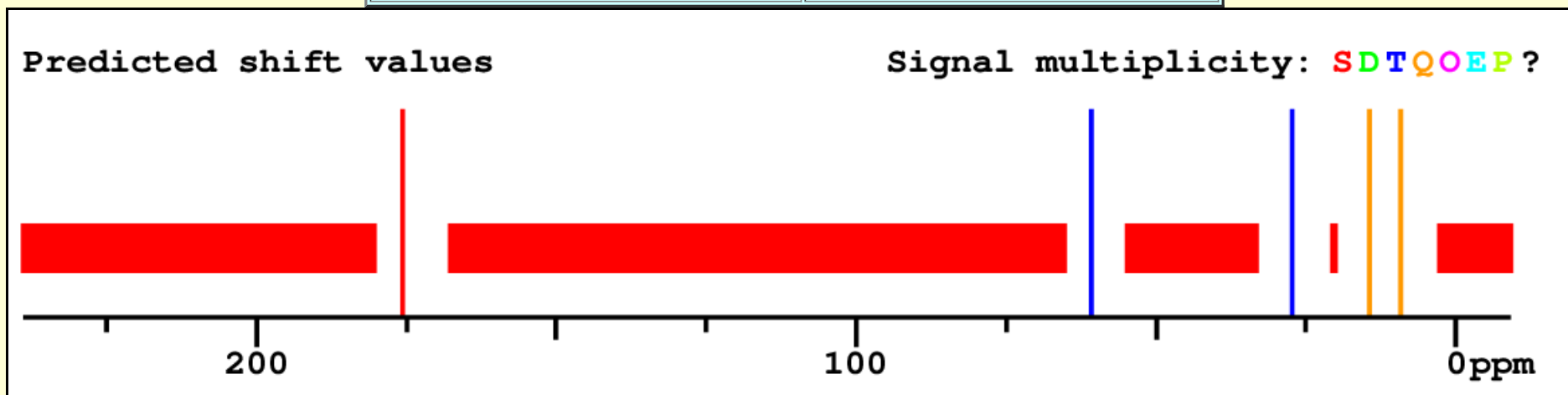
Structure Proposal #1

Structure	Similarity Measure
	Deviation = 0.87 ppm Similarity = 100 % $C_5H_{10}O_2$ MWT = 102.06 Search Web for this structure: FKRCODPIKNYEAC Availability
Predicted Chemical Shiftvalues	Matching Map



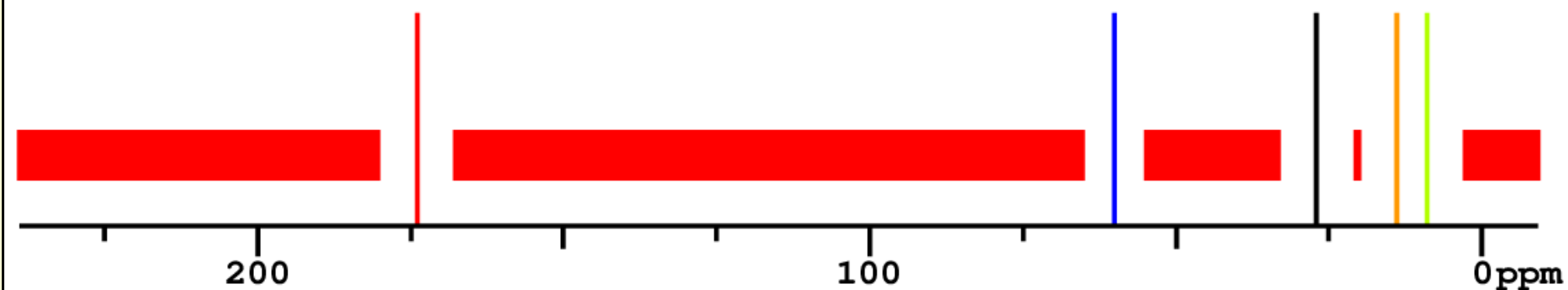
Structure Proposal #2

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



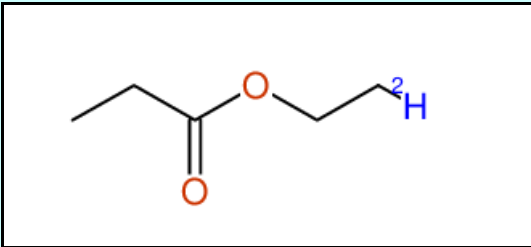
Experimental shift values

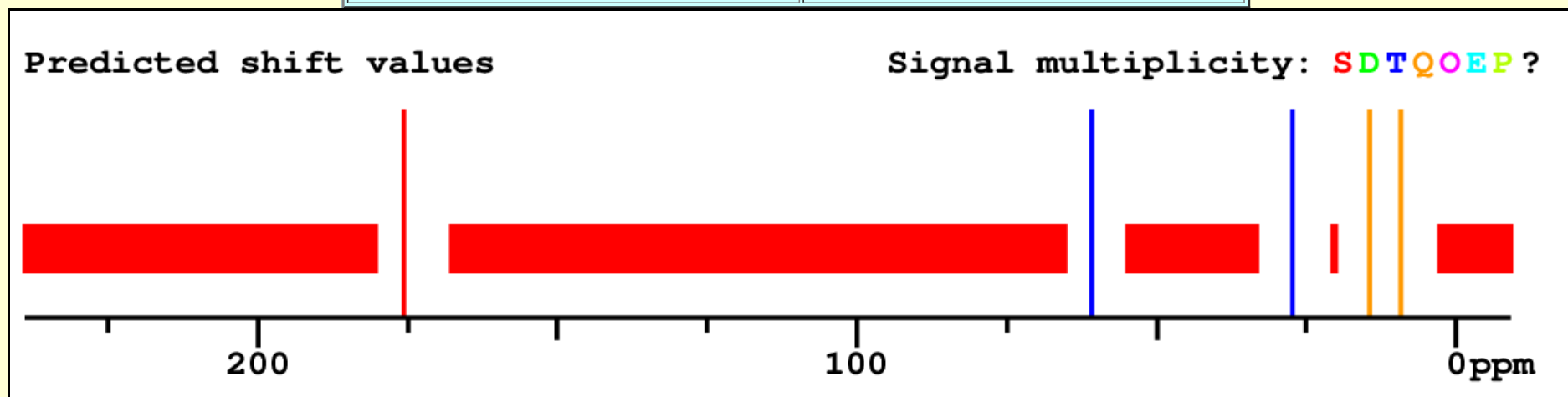
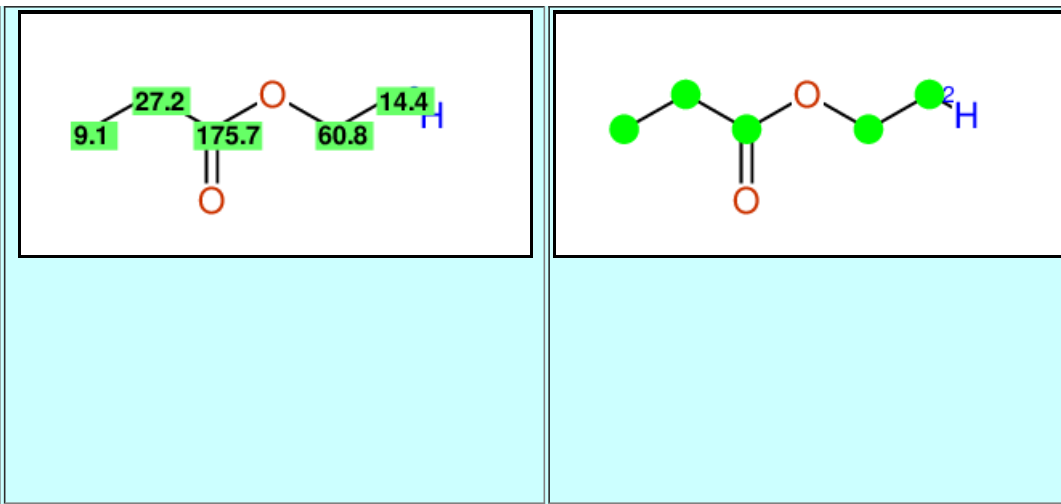
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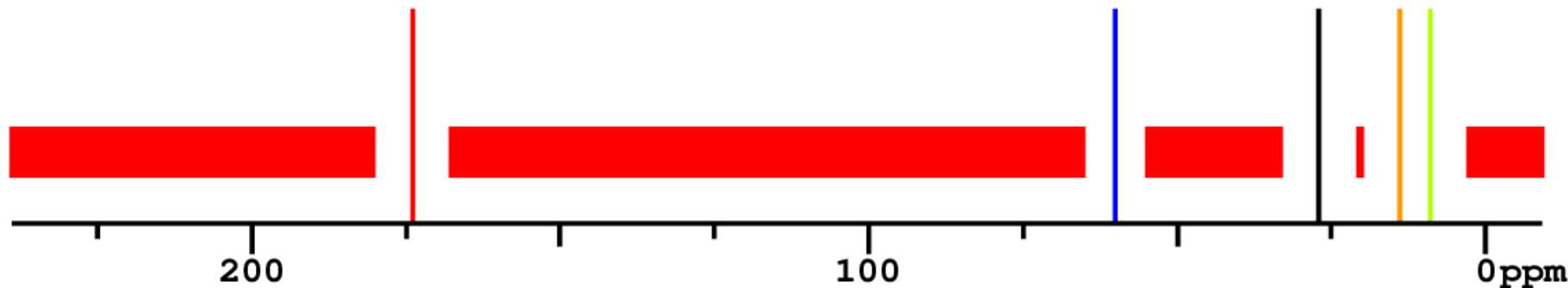
Structure Proposal #3

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



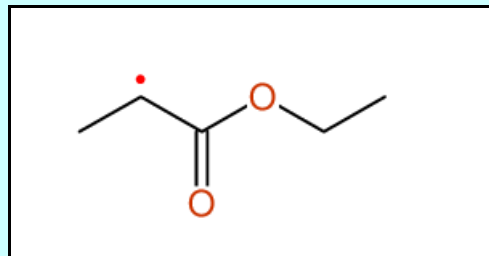
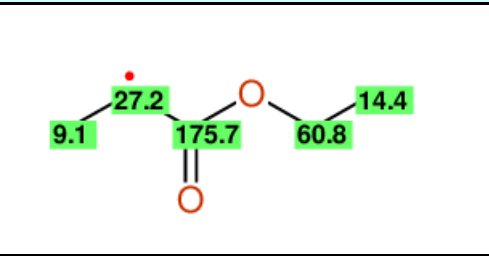
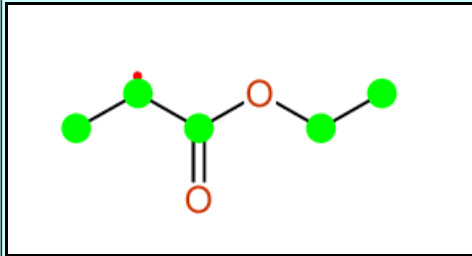
Experimental shift values

No line in reference: 



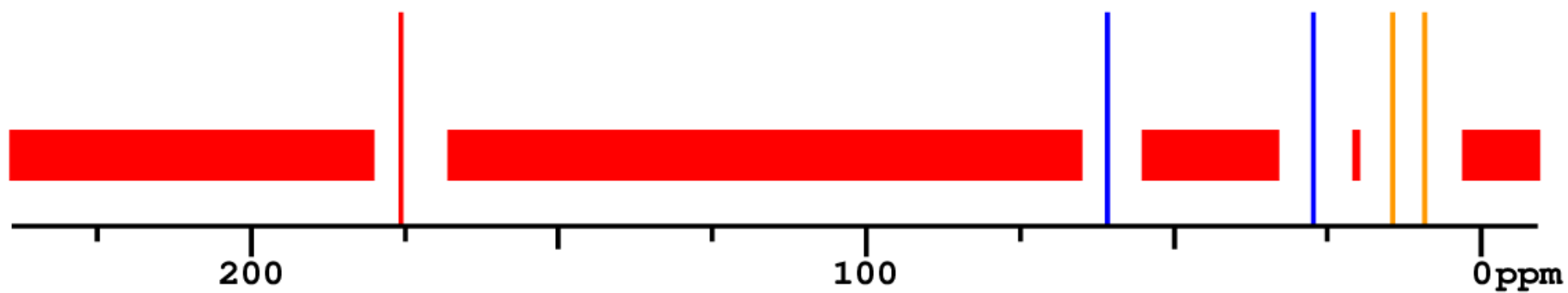
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Structure Proposal #4

Structure	Similarity Measure
	Deviation = 0.87 ppm Similarity = 100 % C ₅ H ₉ O ₂ MWT = 101.06 Search Web for this structure: UPRLWNPAOPKPCE
Predicted Chemical Shiftvalues	Matching Map
	

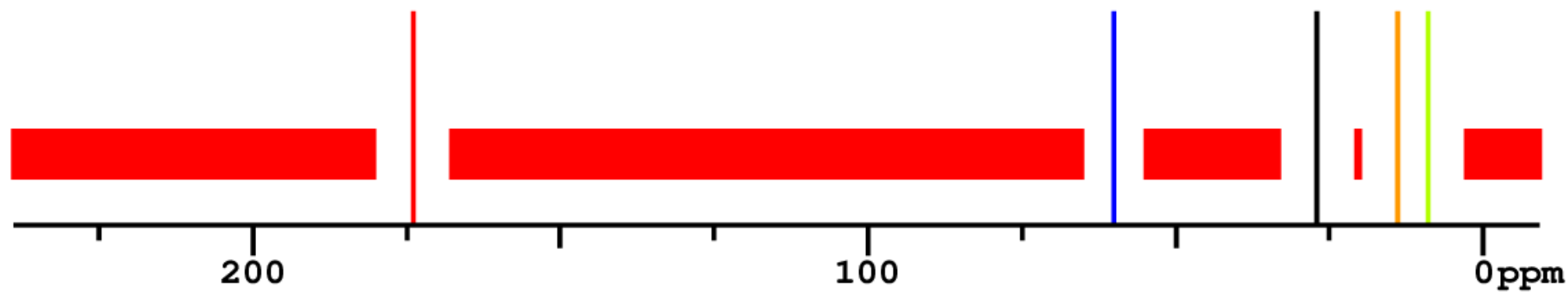
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

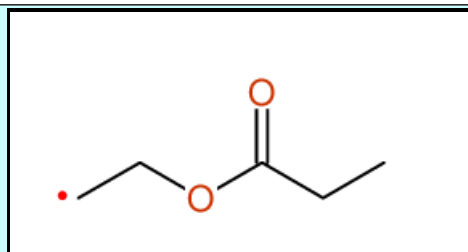
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Structure Proposal #5

Structure	Similarity Measure



Deviation = 0.87 ppm
Similarity = 100 %

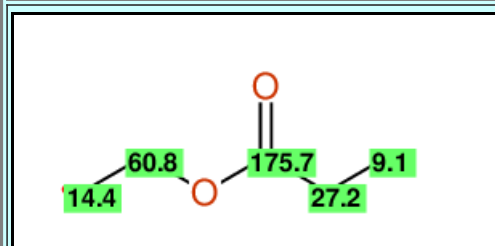
$C_5H_9O_2$

MWT = 101.06

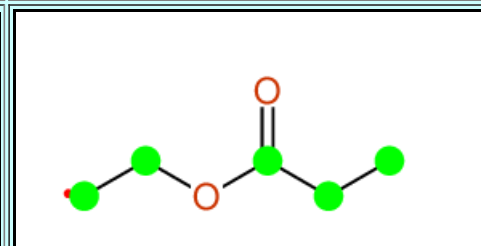
Search Web for this structure:

[IRGLFRDZYNBBCO](#)

Predicted Chemical Shiftvalues

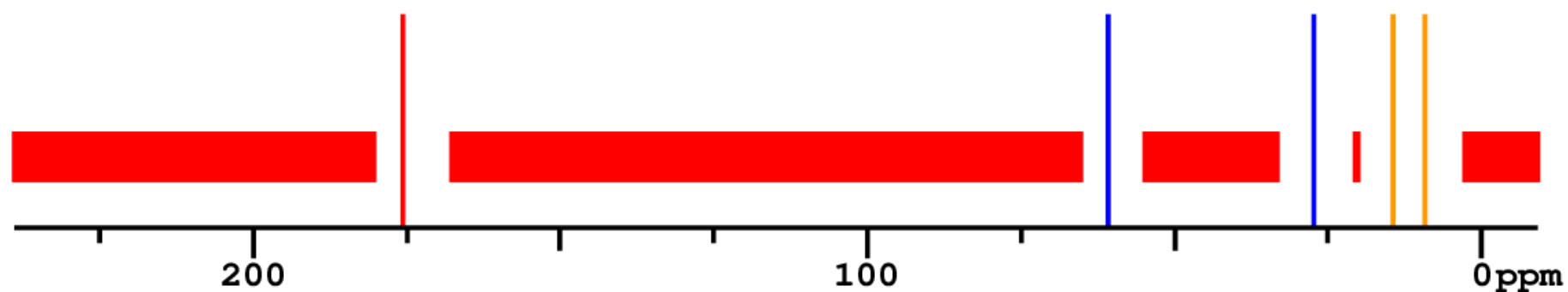


Matching Map



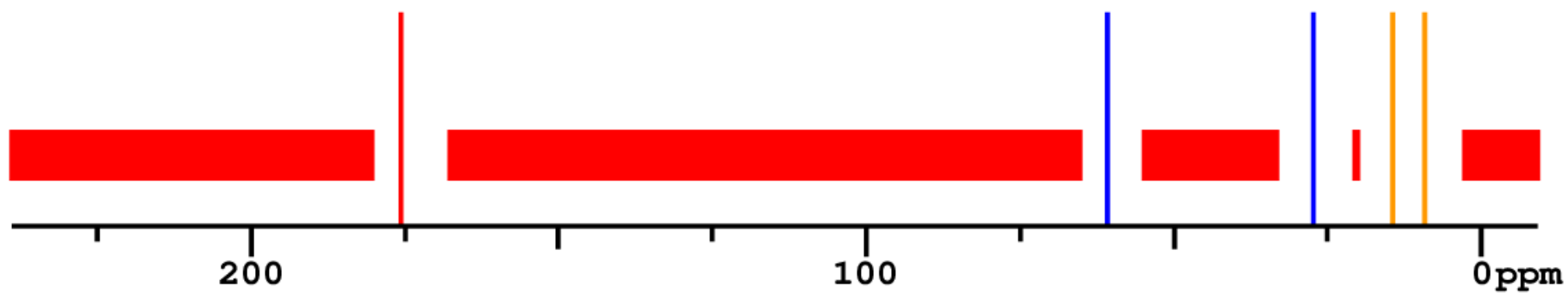
Predicted shift values

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



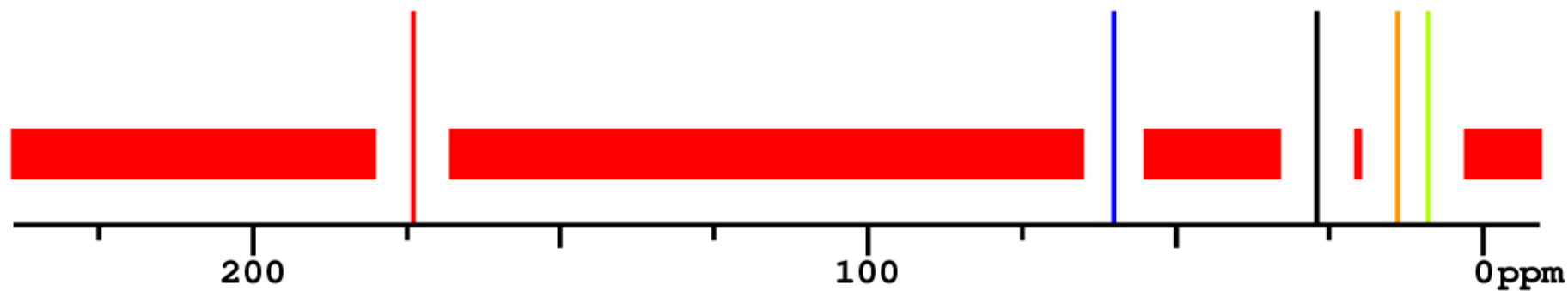
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

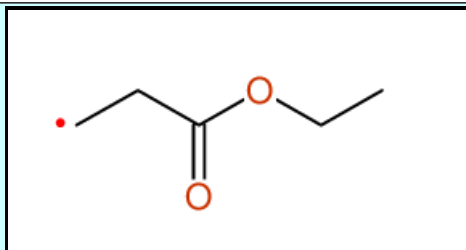
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Structure Proposal #7

Structure	Similarity Measure



Deviation = 0.87 ppm
Similarity = 100 %

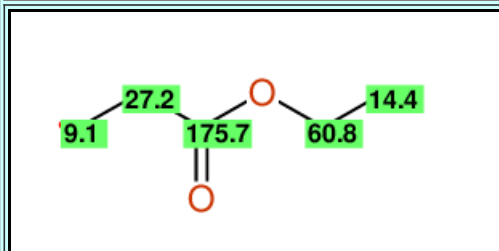
$C_5H_9O_2$

MWT = 101.06

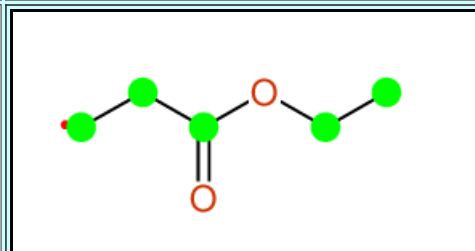
Search Web for this structure:

[SOKCNILPAQLIRC](#)

Predicted Chemical Shiftvalues

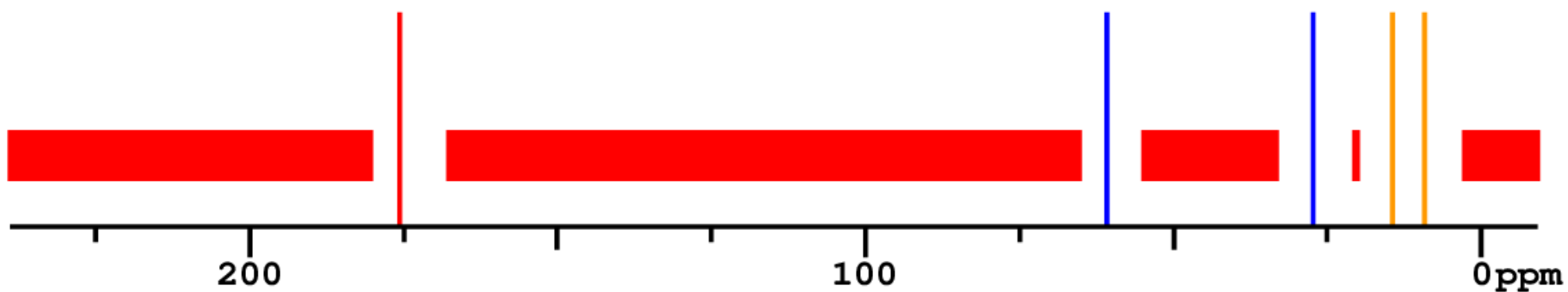


Matching Map



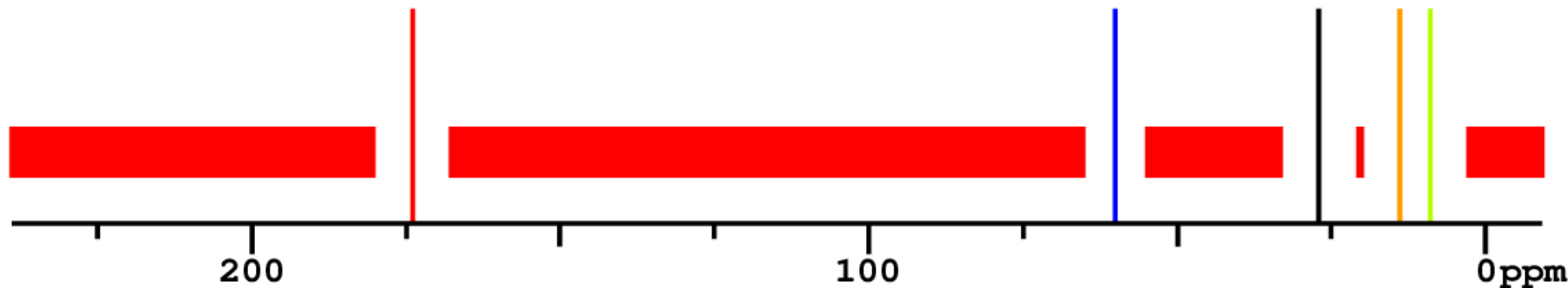
Predicted shift values

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



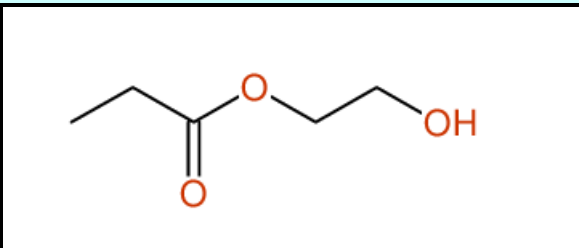
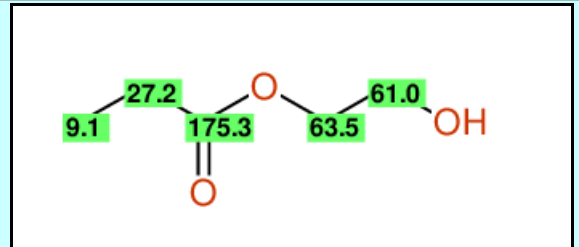
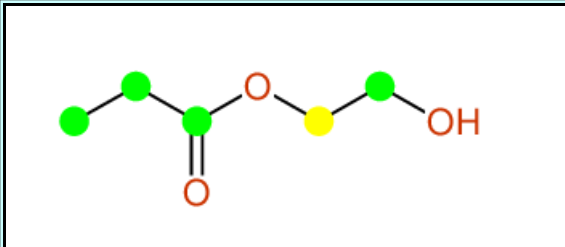
Experimental shift values

No line in reference: 



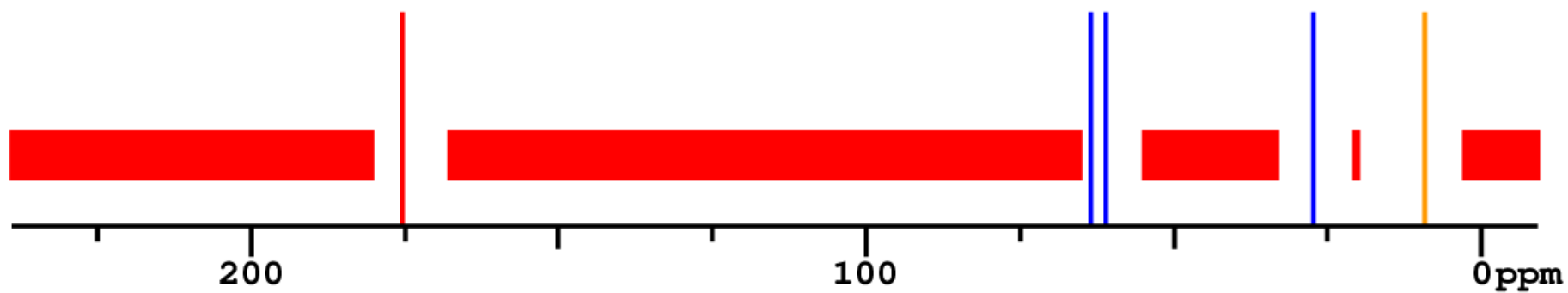
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Structure Proposal #8

Structure	Similarity Measure
	<p>Deviation = 2.02 ppm Similarity = 90 %</p> <p>$C_5H_{10}O_3$</p> <p>MWT = 118.06</p> <p>Search Web for this structure: SFAMKDPMPDEXGH</p>
Predicted Chemical Shiftvalues	Matching Map
	

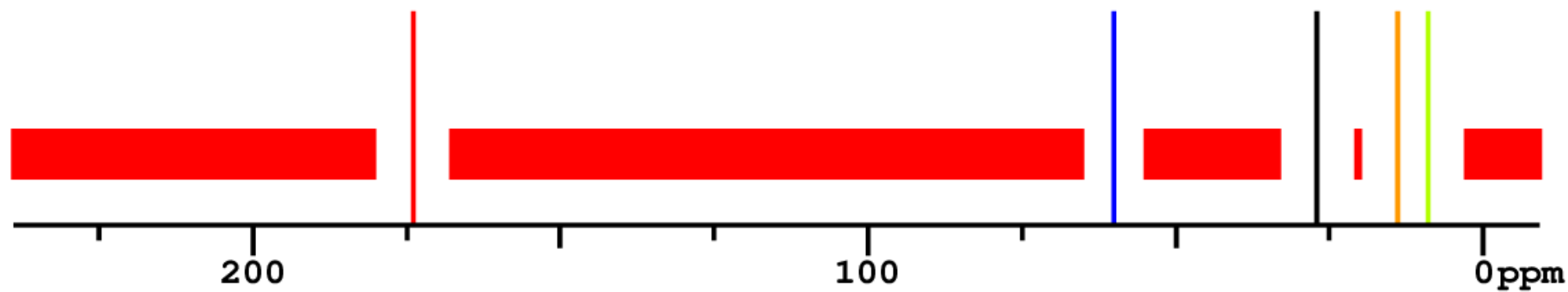
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

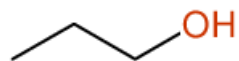
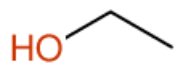
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Structure Proposal #9

Structure	Similarity Measure



Deviation = 2.62 ppm
Similarity = 90 %

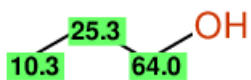
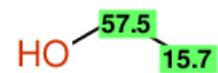
$C_3H_8O \cdot C_2H_6O$

MWT = 106.06

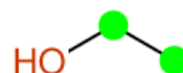
Search Web for this
structure:

[OMRDZQXXMYCHBU](#)

Predicted Chemical
Shiftvalues

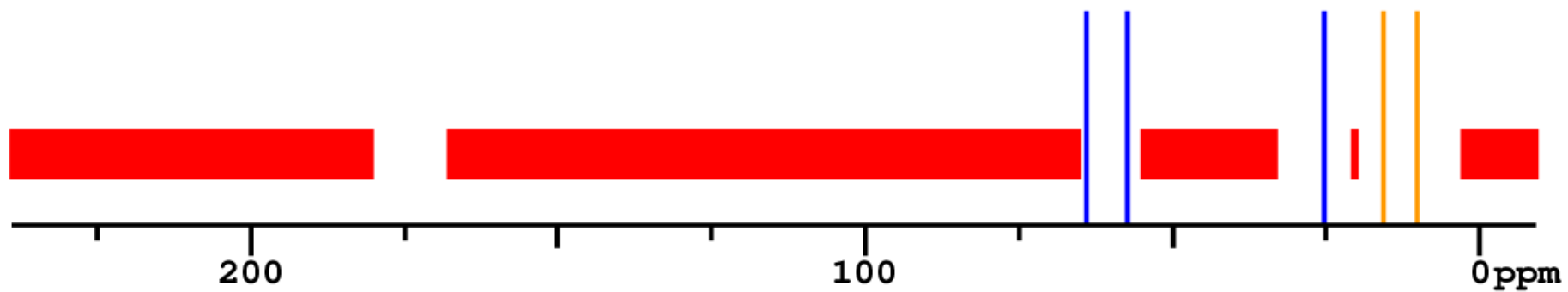


Matching Map



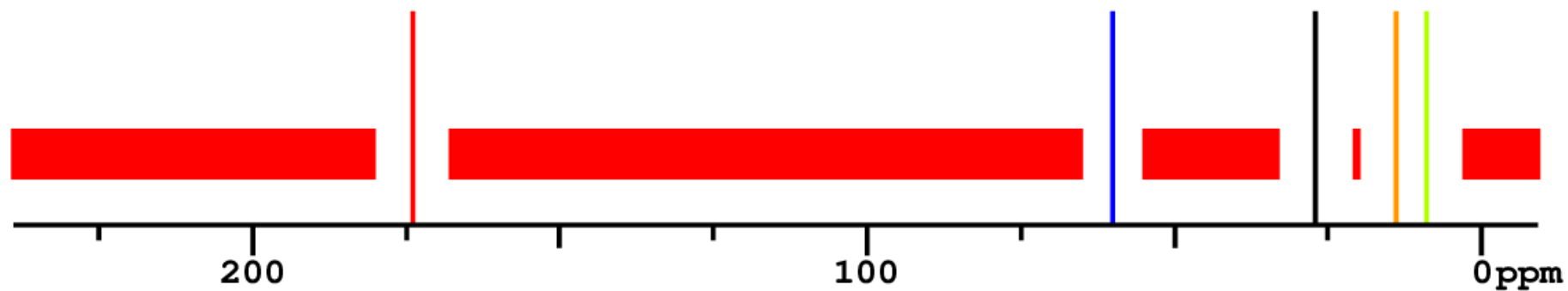
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

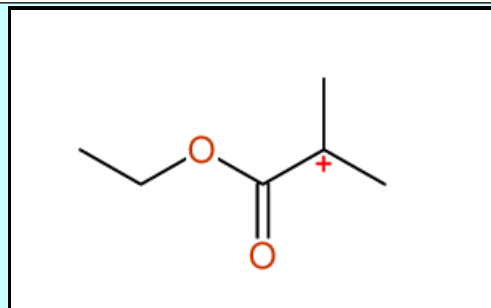
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Structure Proposal #10

Structure	Similarity Measure



Deviation = 2.93 ppm
Similarity = 100 %

$C_6H_{11}O_2$

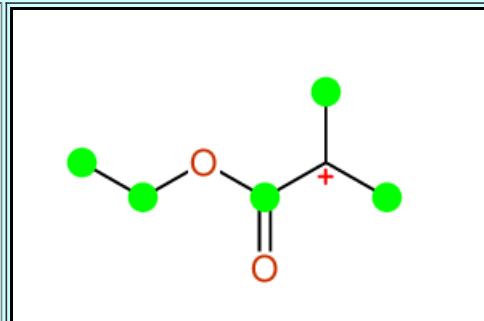
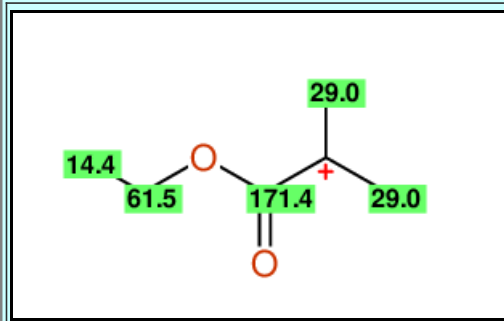
MWT = 115.07

Search Web for this structure:

[BNJCQKCNZHKCSE](#)

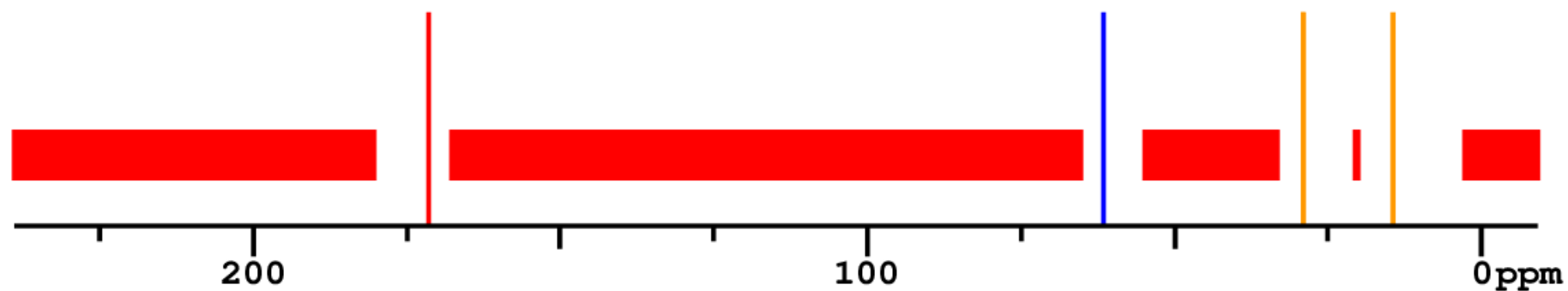
Predicted Chemical Shiftvalues

Matching Map




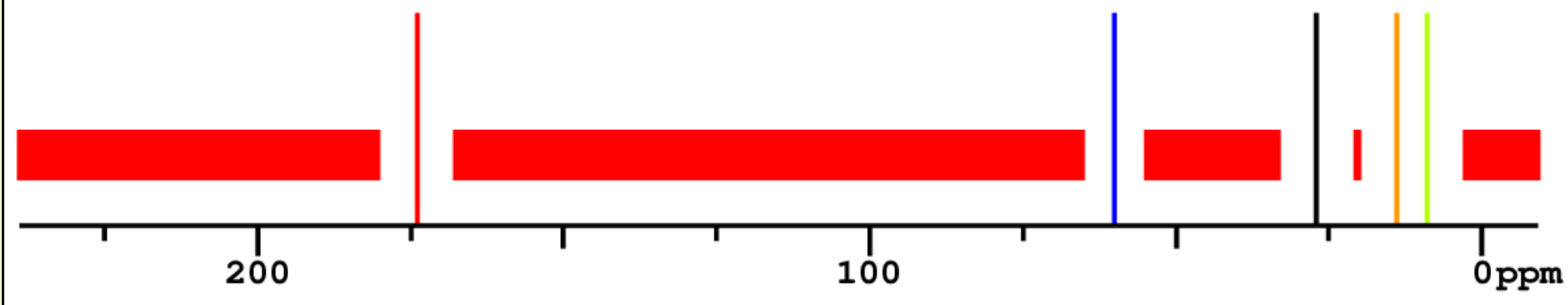
Predicted shift values

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



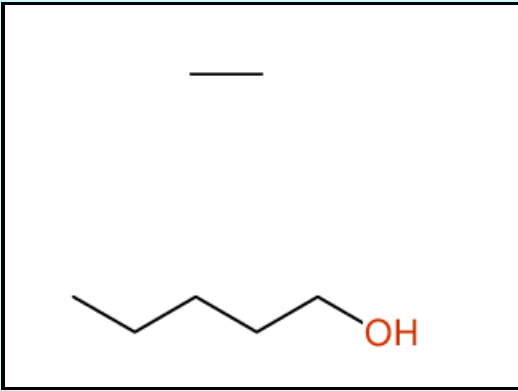
Experimental shift values

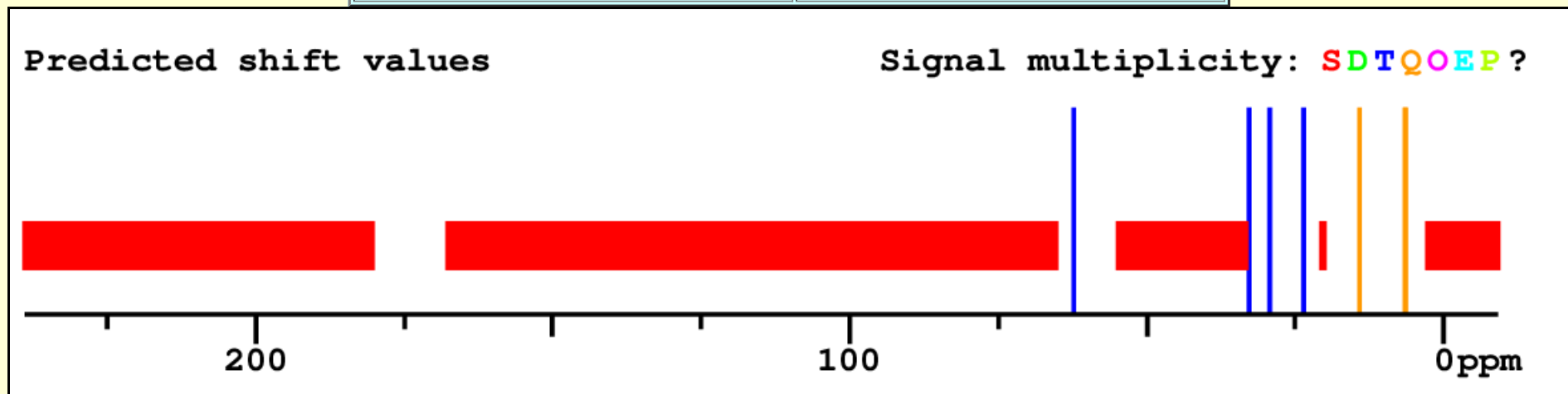
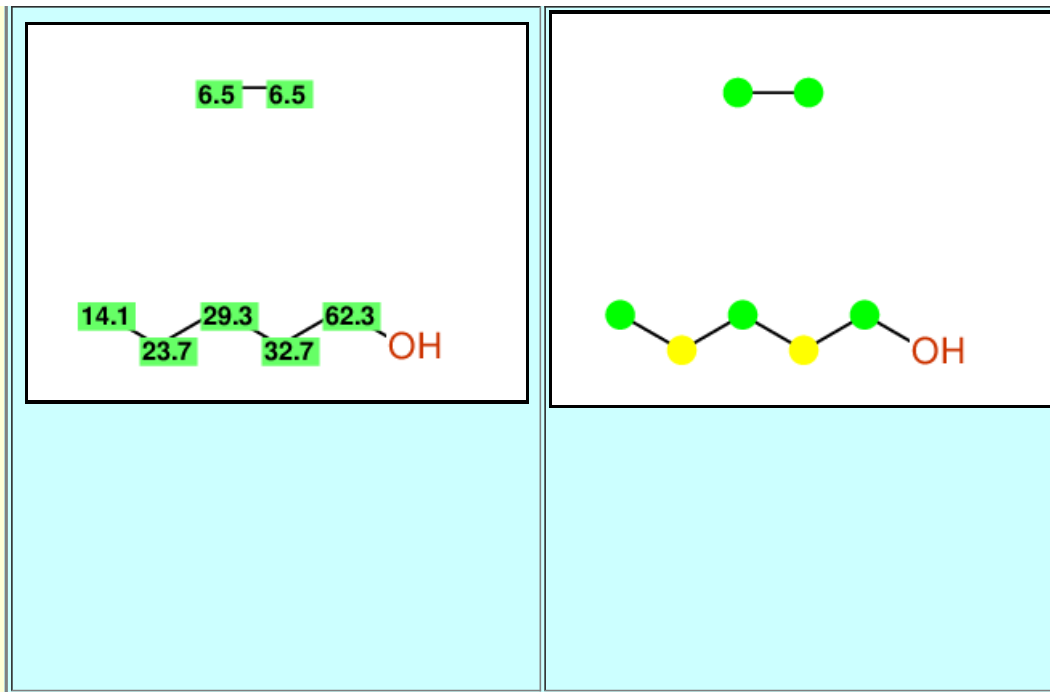
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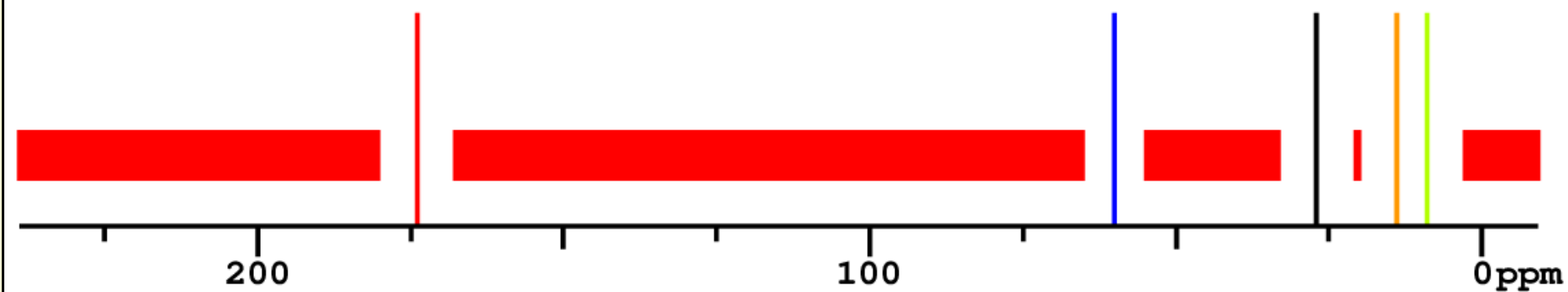
Structure Proposal #11

Structure	Similarity Measure
	<p>Deviation = 2.98 ppm Similarity = 86 %</p> <p>$C_5H_{12}O \cdot C_2H_6$</p> <p>MWT = 118.08</p> <p>Search Web for this structure: ZARMDFHJSIZKO</p>
Predicted Chemical Shiftvalues	Matching Map



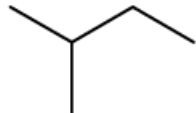
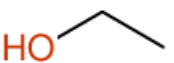
Experimental shift values

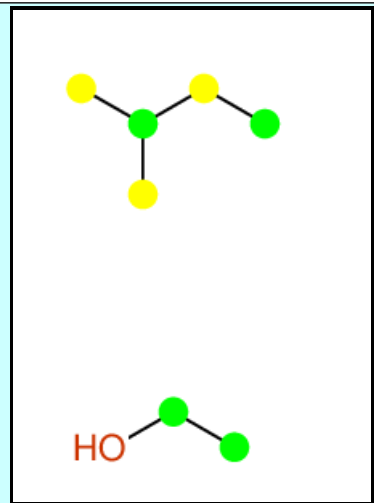
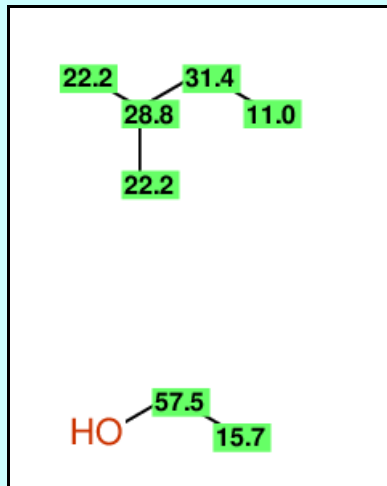
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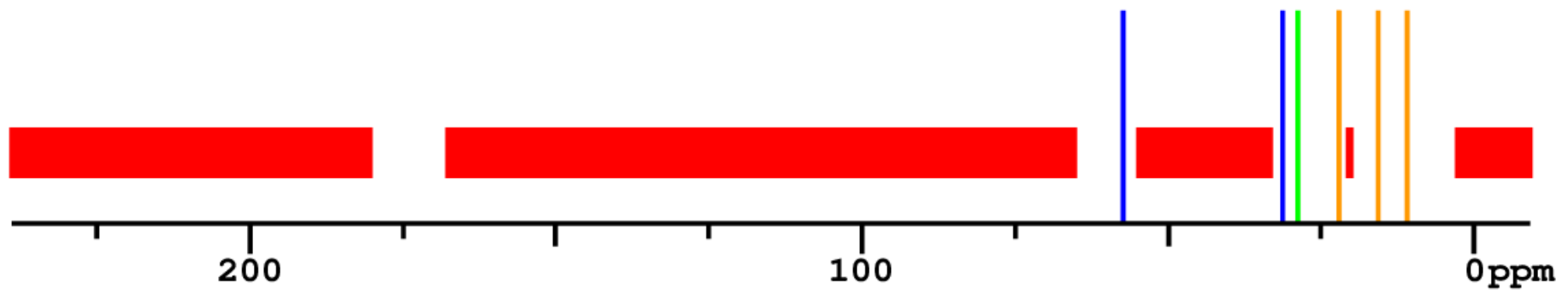
Structure Proposal #12

Structure	Similarity Measure
 	Deviation = 3.16 ppm Similarity = 79 % $C_5H_{12} \cdot C_2H_6O$ MWT = 118.08 Search Web for this structure: FOXQTCHXXJKLNK
Predicted Chemical Shiftvalues	Matching Map




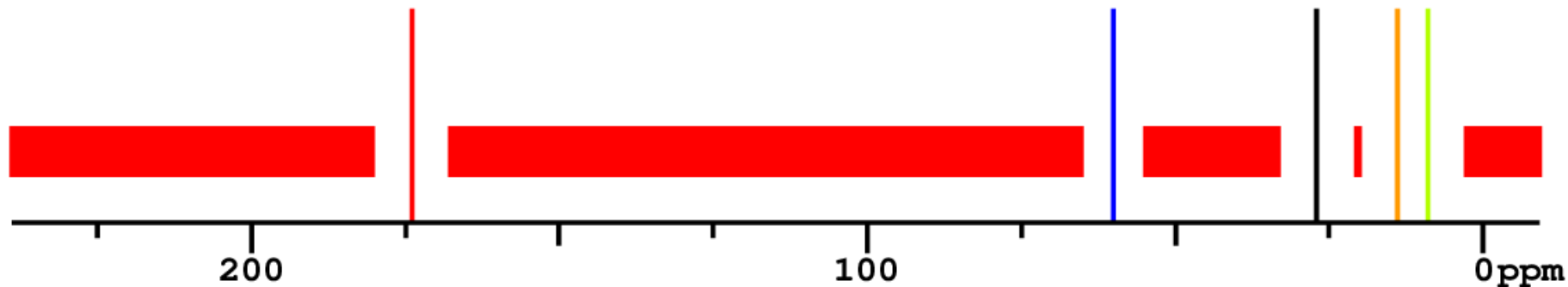
Predicted shift values

Signal multiplicity: S D T Q O E P ?



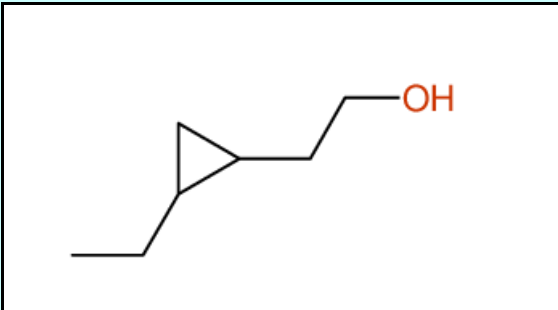
Experimental shift values

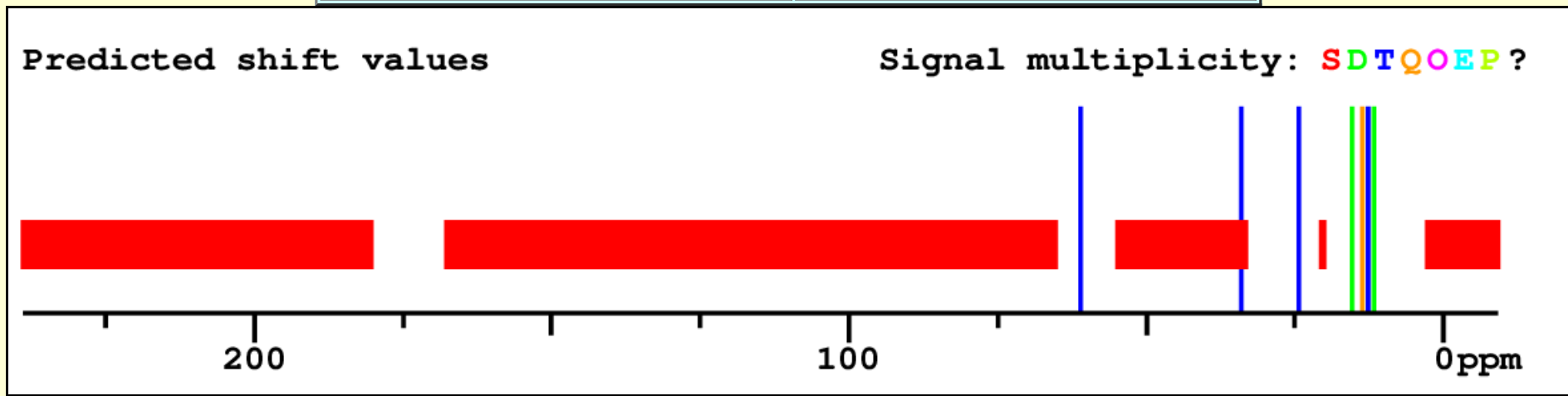
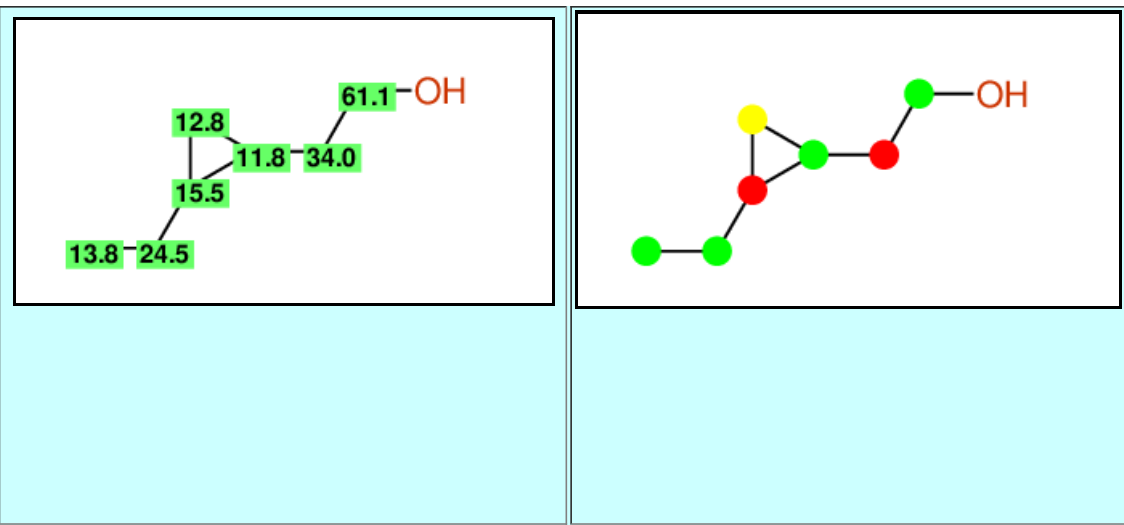
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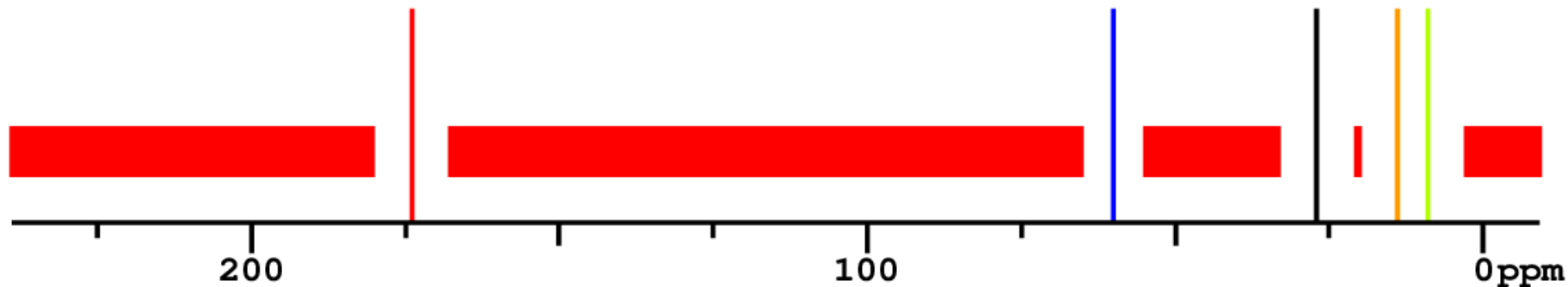
Structure Proposal #13

Structure	Similarity Measure
	<p>Deviation = 3.49 ppm Similarity = 64 % (Different pattern)</p> <p>$C_7H_{14}O$</p> <p>MWT = 114.08</p> <p>Search Web for this structure: IPKMDCPNAOYUEB</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



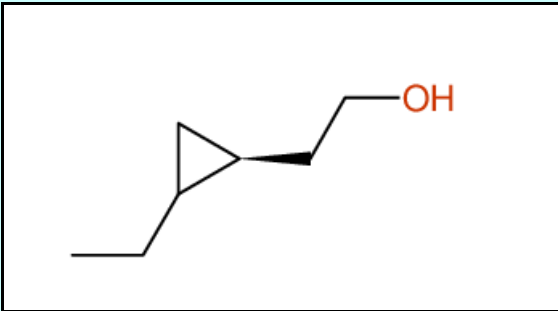
Experimental shift values

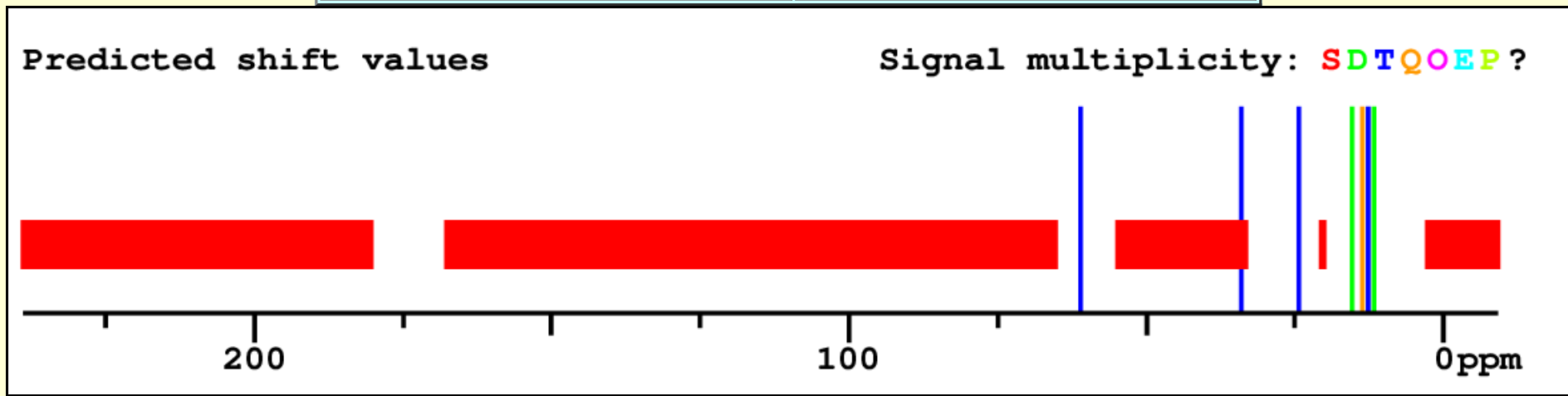
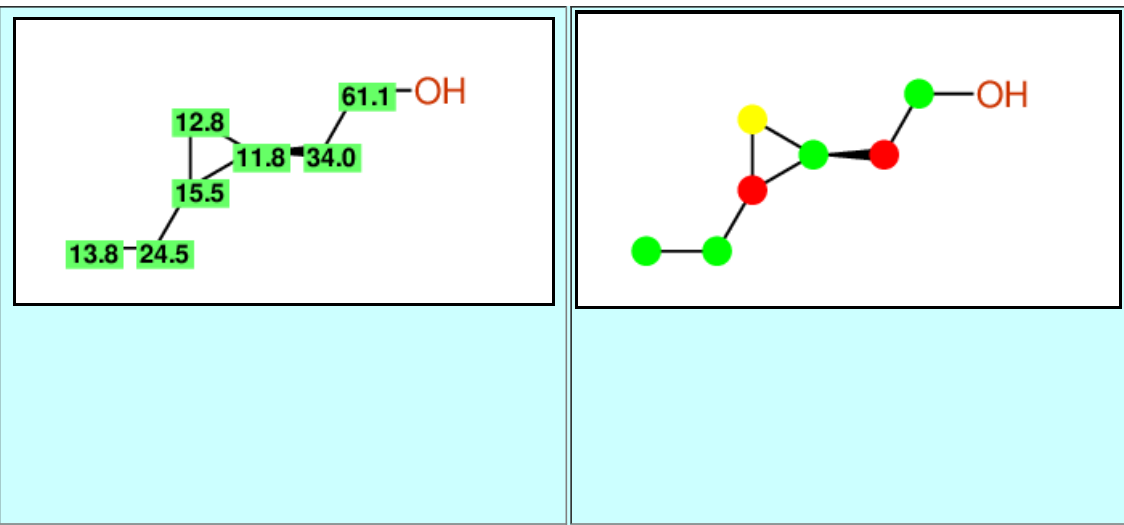
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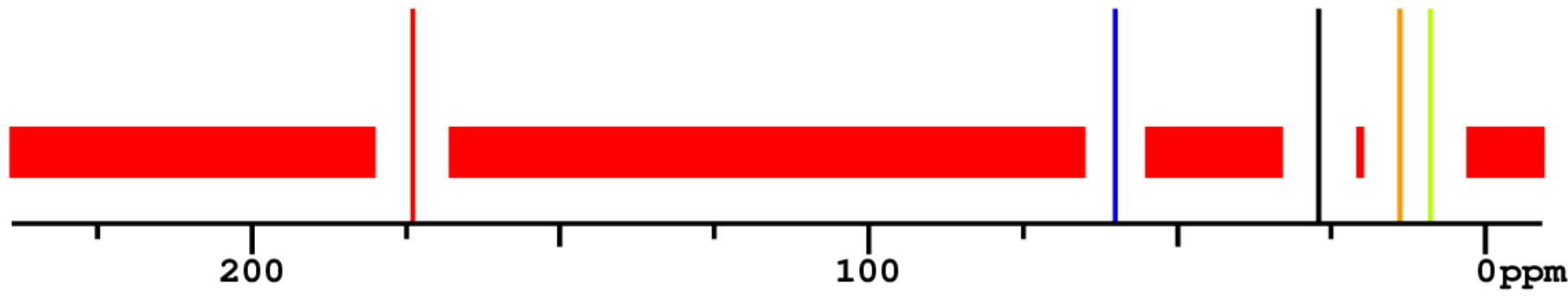
Structure Proposal #14

Structure	Similarity Measure
	<p>Deviation = 3.49 ppm Similarity = 64 % (Different pattern)</p> <p>$C_7H_{14}O$</p> <p>MWT = 114.08</p> <p>Search Web for this structure: IPKMDCPNAOYUEB</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



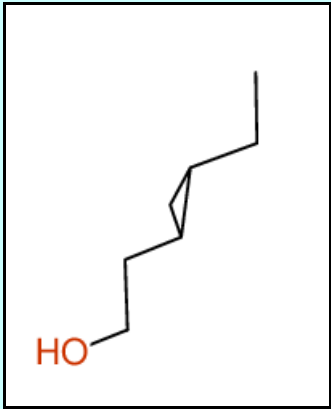
Experimental shift values

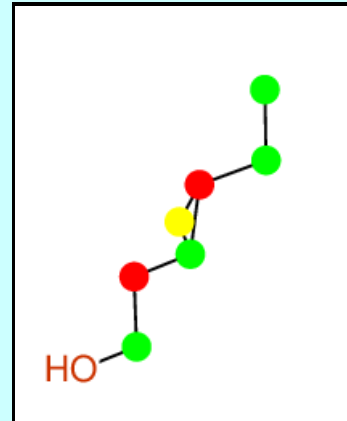
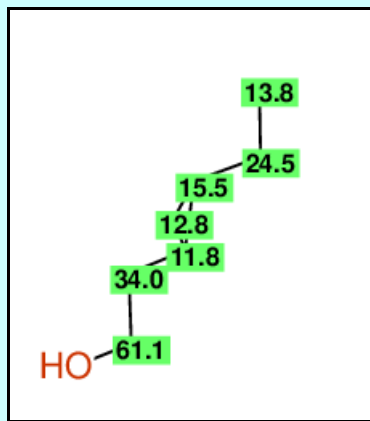
No line in reference: 



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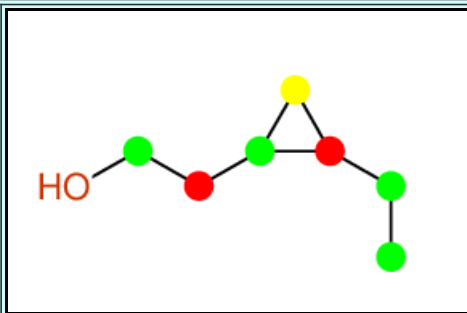
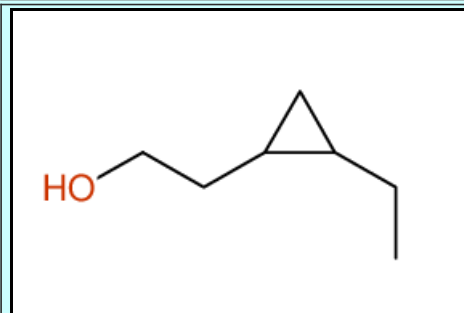
Structure Proposal #15

Structure	Similarity Measure
	<p>Deviation = 3.49 ppm Similarity = 64 % (Different pattern)</p> <p>$C_7H_{14}O$</p> <p>MWT = 114.08</p> <p>Search Web for this structure: IPKMDCPNAOYUEB Availability</p>
Predicted Chemical Shiftvalues	Matching Map



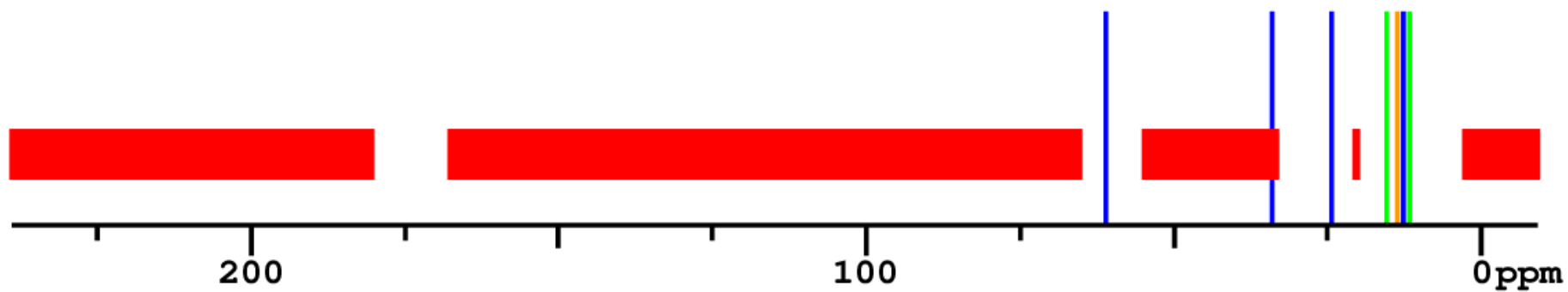
2D Structure Representation

2D Matching Map



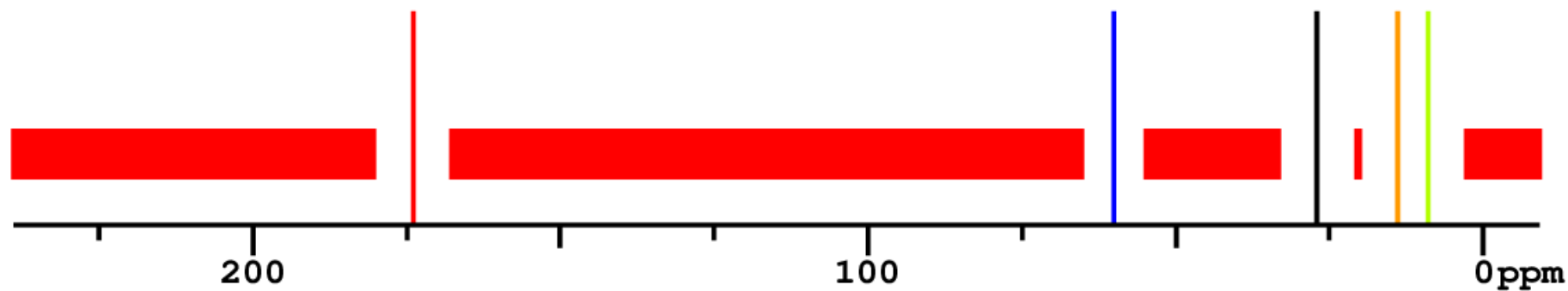
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

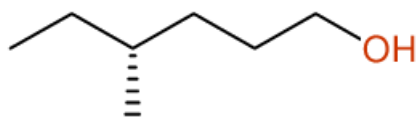
No line in reference: [red bar]



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Structure Proposal #16

Structure	Similarity Measure



Deviation = 4.01 ppm
 Similarity = 50 %
 (Different pattern)

$C_7H_{16}O$

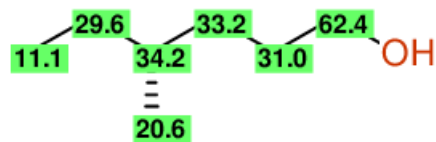
MWT = 116.08

Search Web for this structure:

[YNPVNLWKVZZBTM](#)

[Availability](#)

Predicted Chemical Shiftvalues

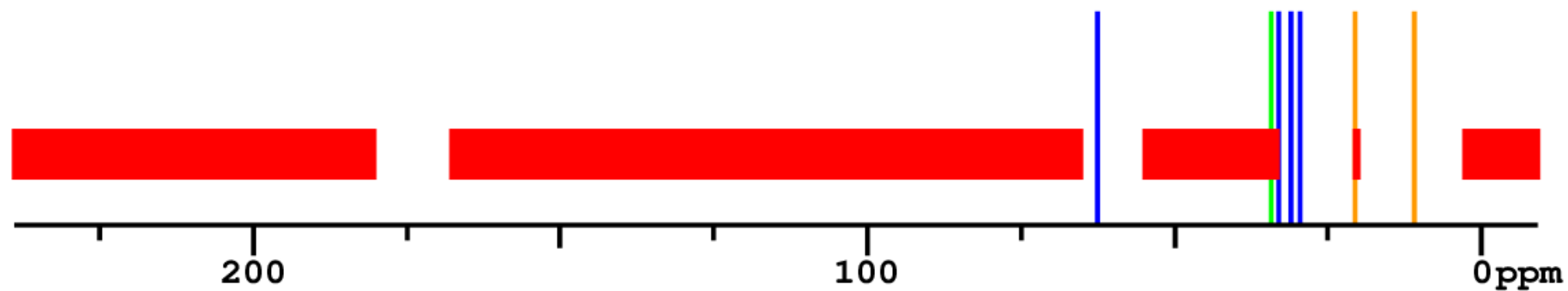


Matching Map



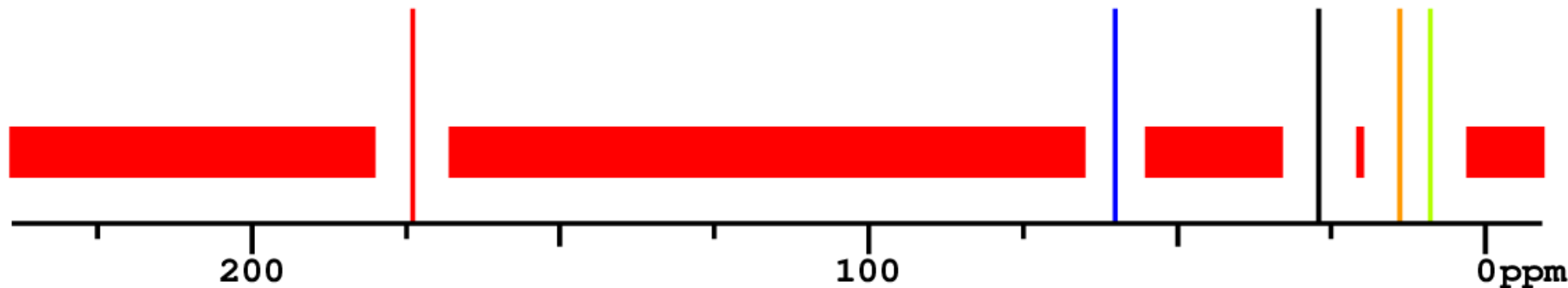
Predicted shift values

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



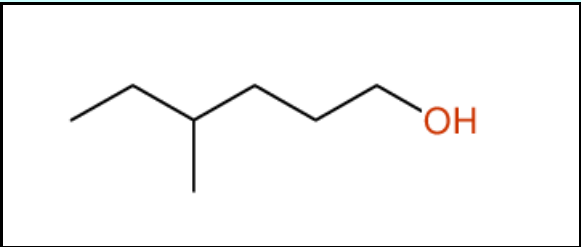
Experimental shift values

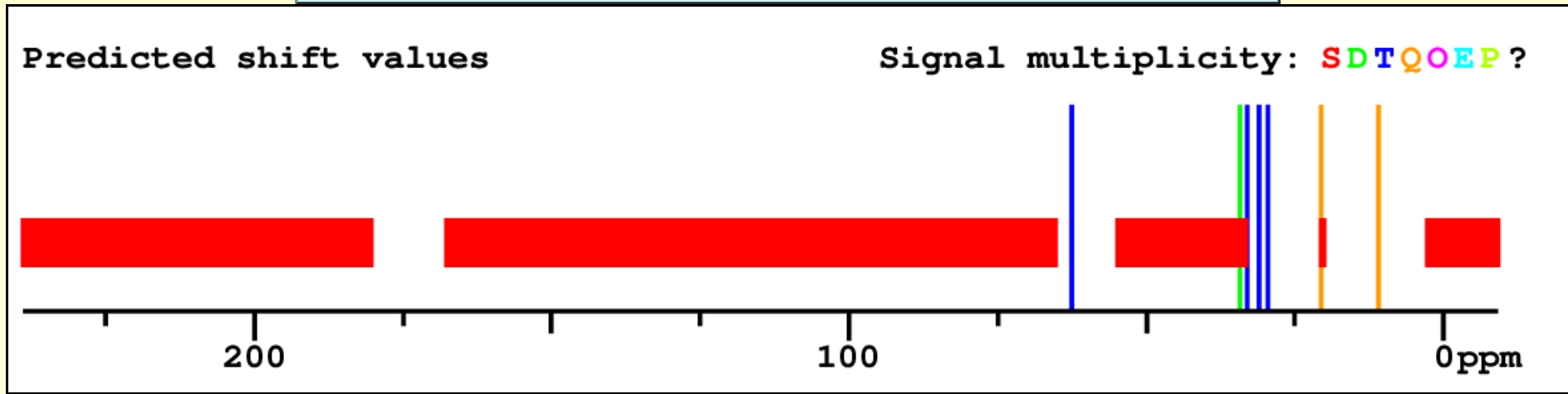
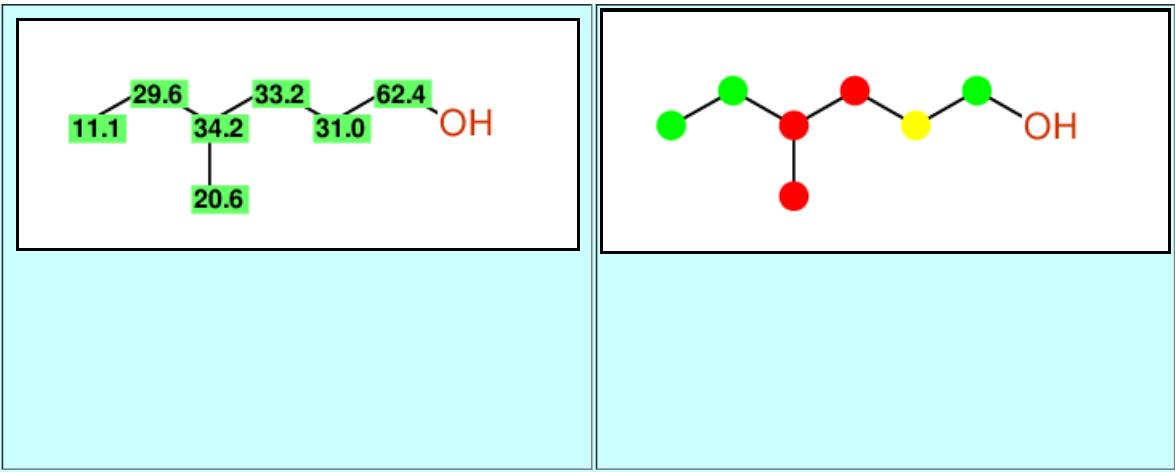
No line in reference: 



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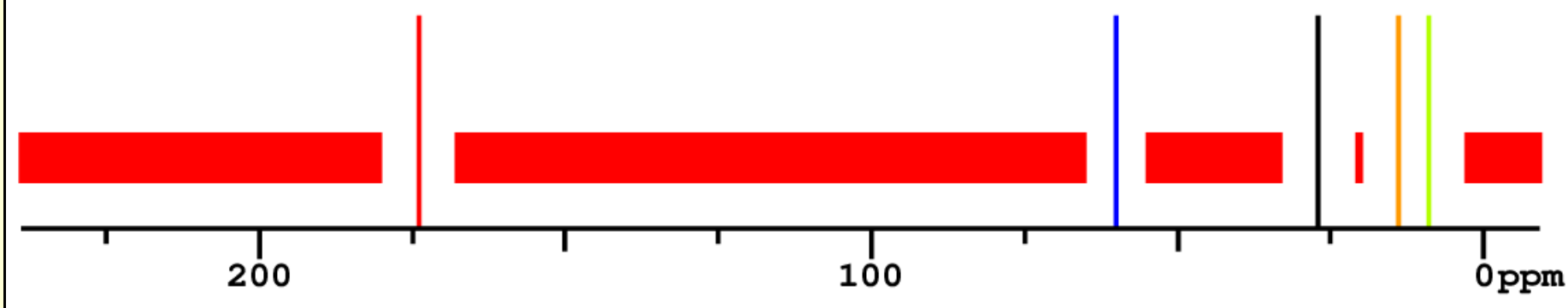
Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 4.01 ppm Similarity = 50 % (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>Search Web for this structure: YNPVNLWKVZZBTM Availability</p>
Predicted Chemical Shiftvalues	Matching Map



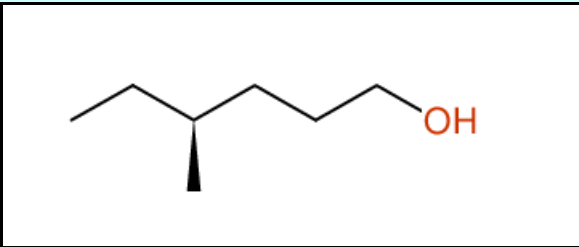
Experimental shift values

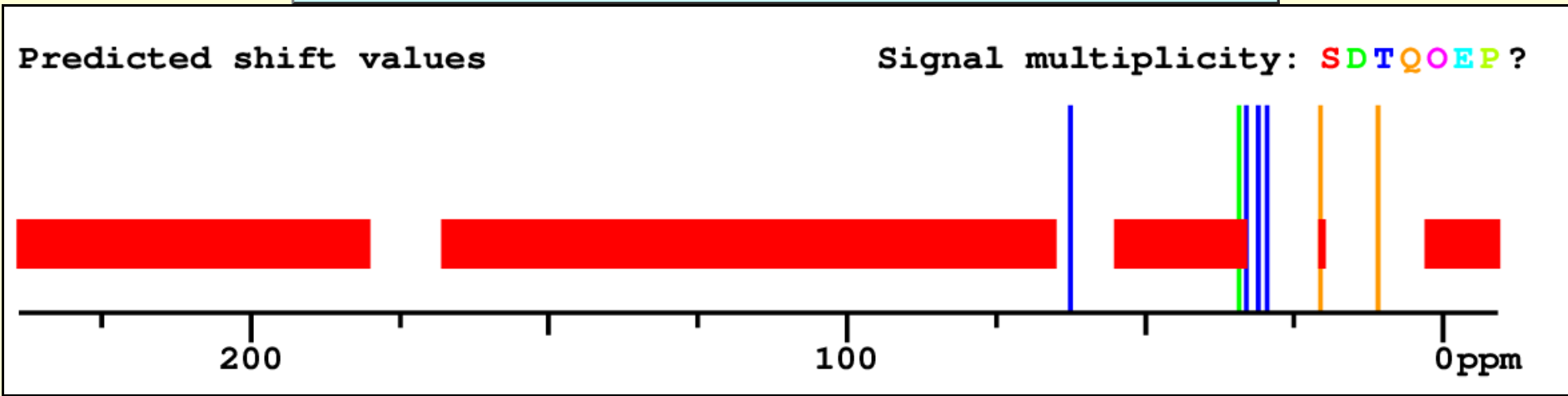
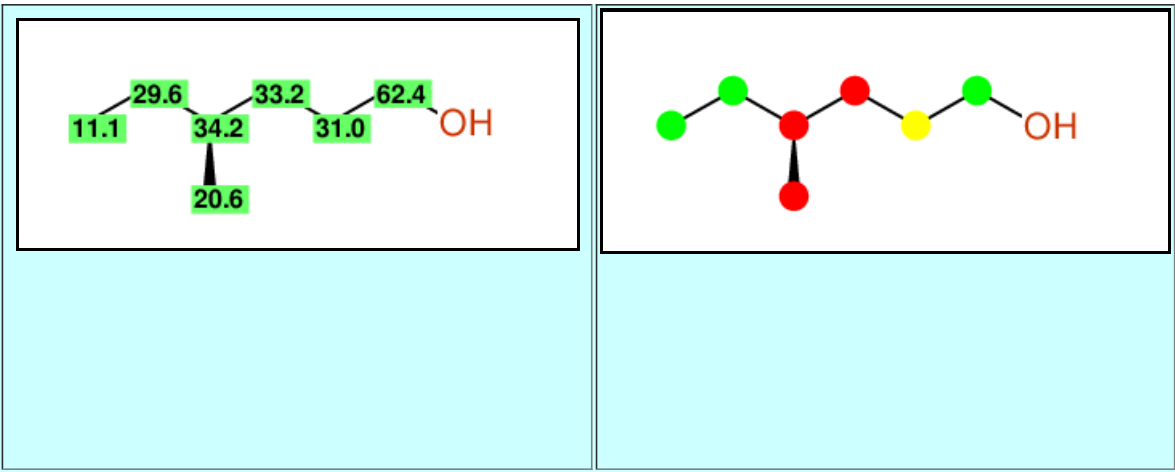
No line in reference: 



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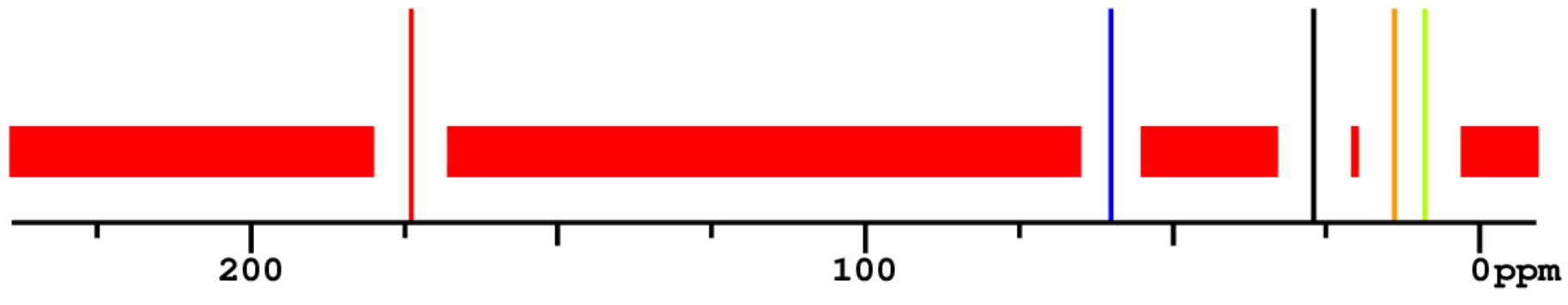
Structure Proposal #18

Structure	Similarity Measure
 <p><chem>CCCC(C)CO</chem></p>	<p>Deviation = 4.01 ppm Similarity = 50 % (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>Search Web for this structure: YNPVNLWKVZZBTM</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



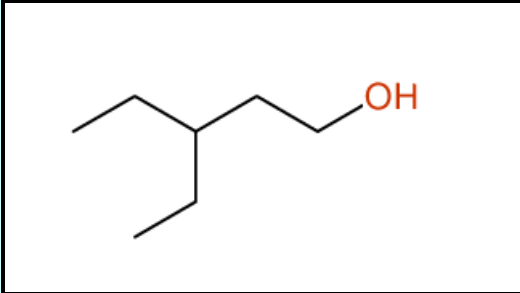
Experimental shift values

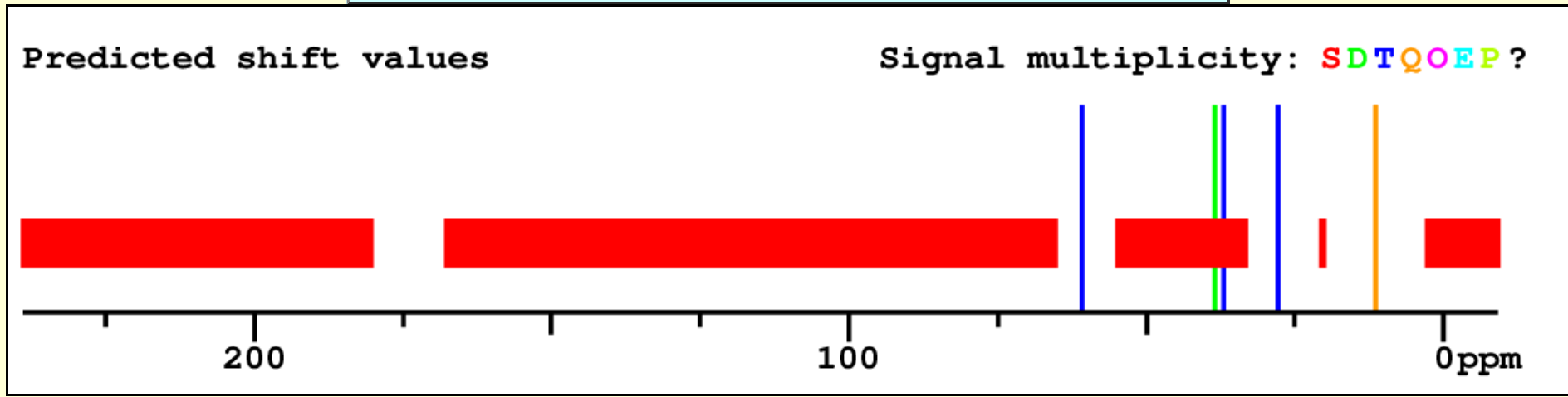
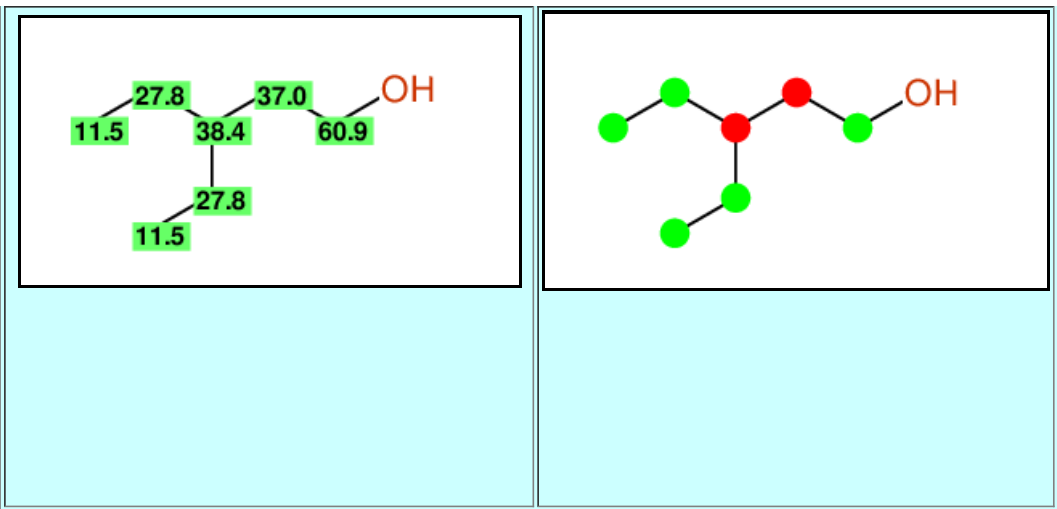
No line in reference: 



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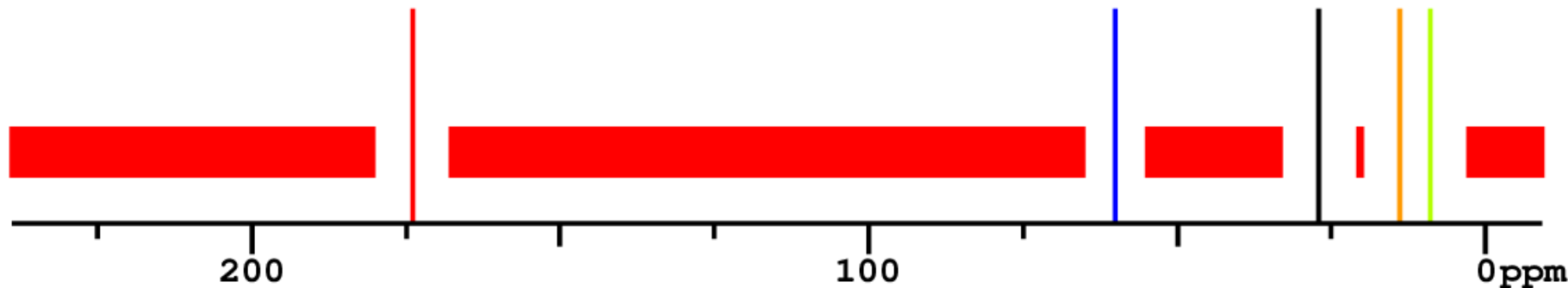
Structure Proposal #19

Structure	Similarity Measure
	<p>Deviation = 4.36 ppm Similarity = 71 % (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 116.08</p> <p>Search Web for this structure: DVEFUHVWJONKR</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



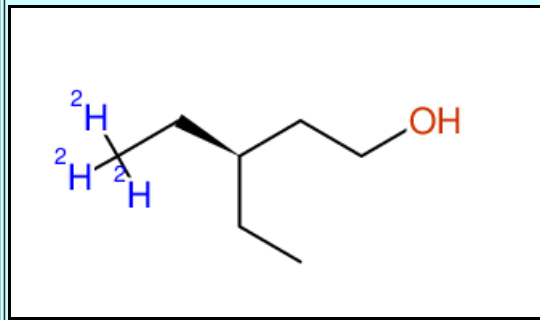
Experimental shift values

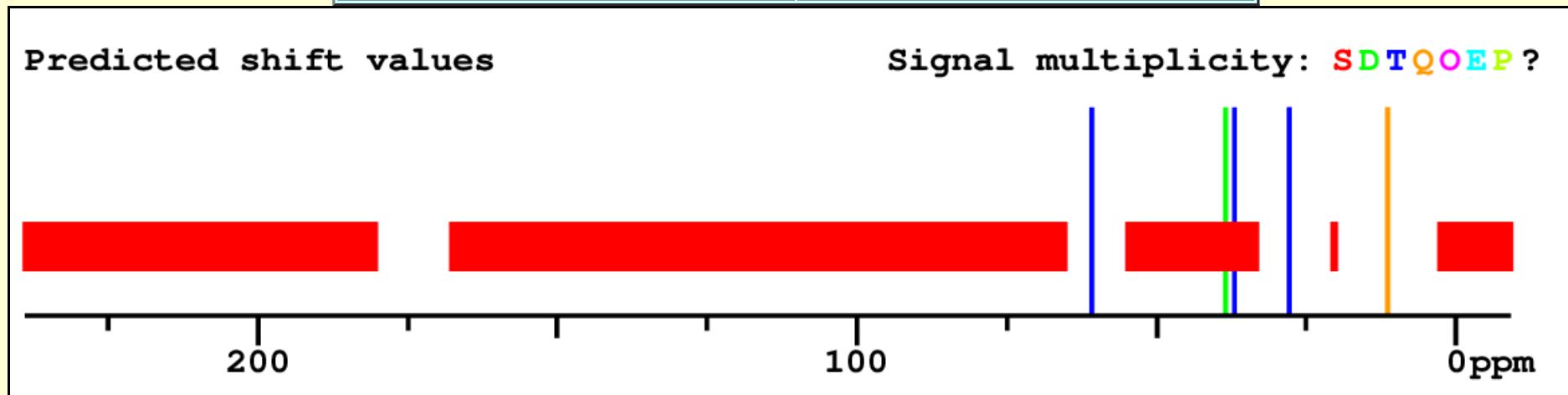
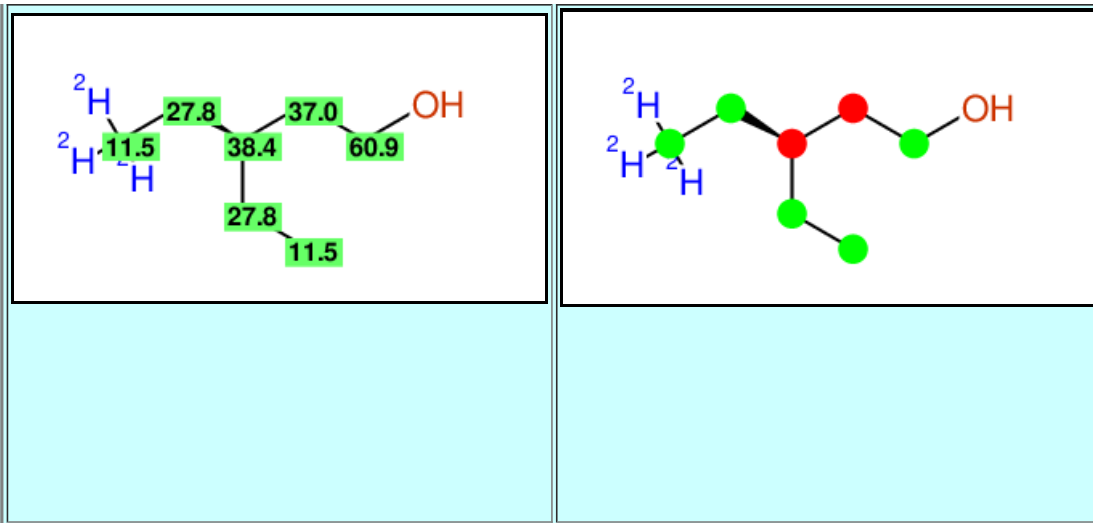
No line in reference: ████████



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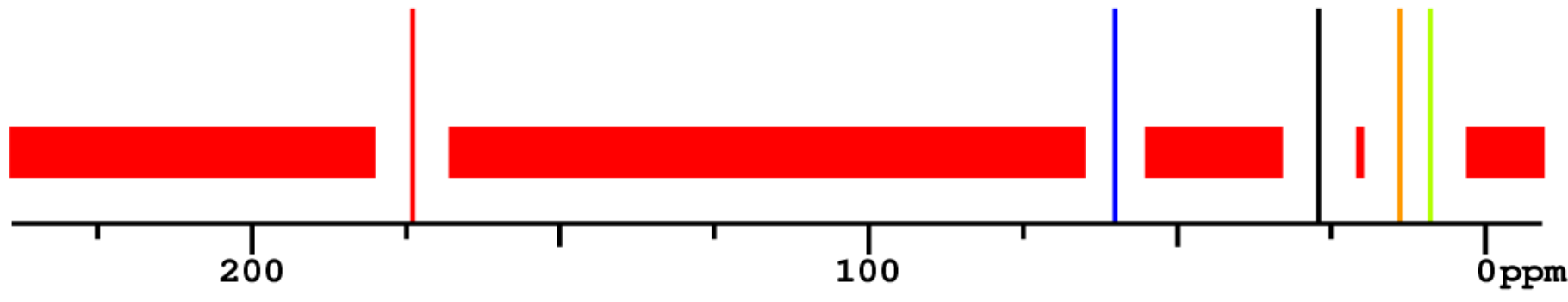
Structure Proposal #20

Structure	Similarity Measure
	<p>Deviation = 4.36 ppm Similarity = 71 % (Different pattern)</p> <p>$C_7H_{16}O$</p> <p>MWT = 119.08</p> <p>Search Web for this structure: DVEFUHVWJONKR</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



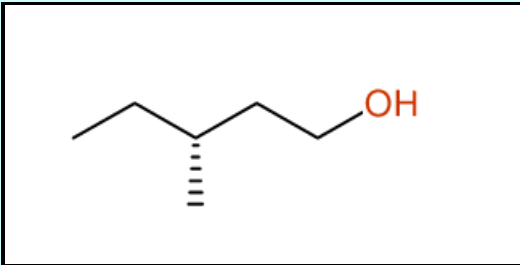
Experimental shift values

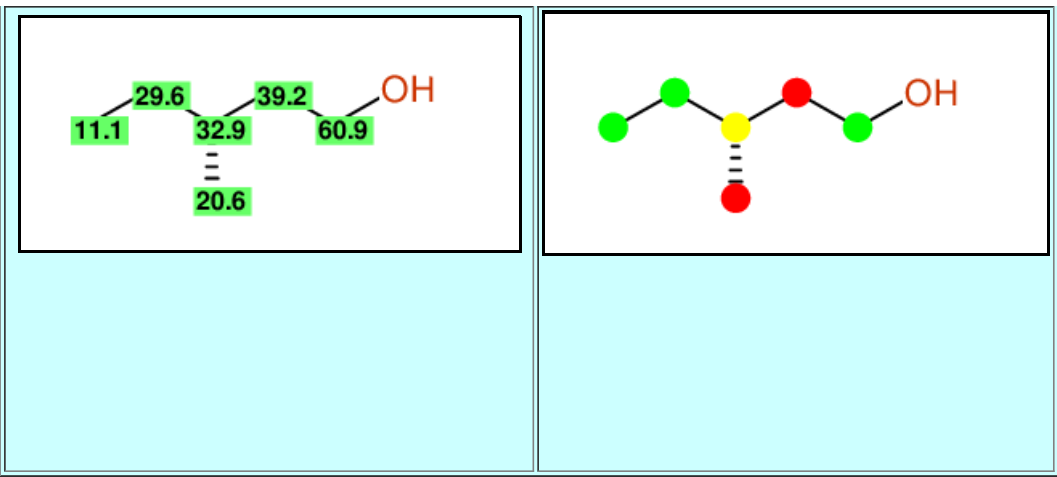
No line in reference: 



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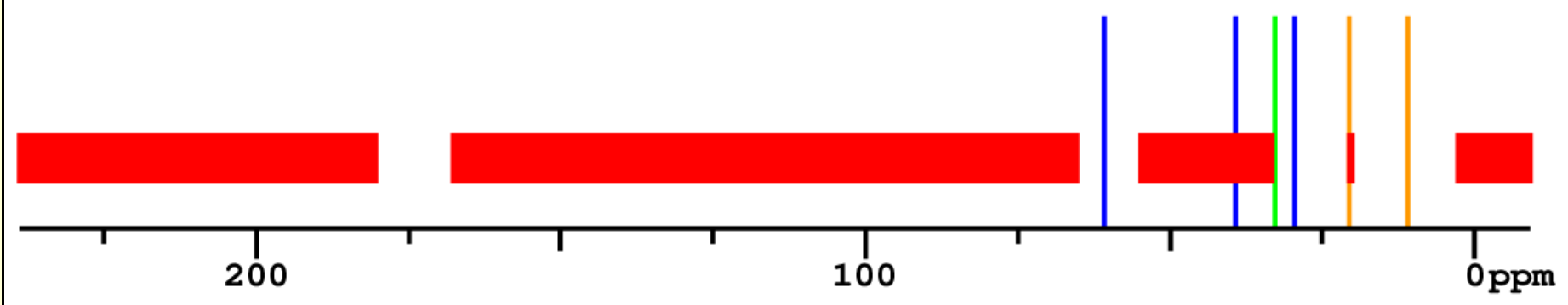
Structure Proposal #21

Structure	Similarity Measure
	<p>Deviation = 4.64 ppm Similarity = 58 % (Different pattern)</p> <p>$C_6H_{14}O$</p> <p>MWT = 102.07</p> <p>Search Web for this structure: IWTVKIGCDZRPL</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



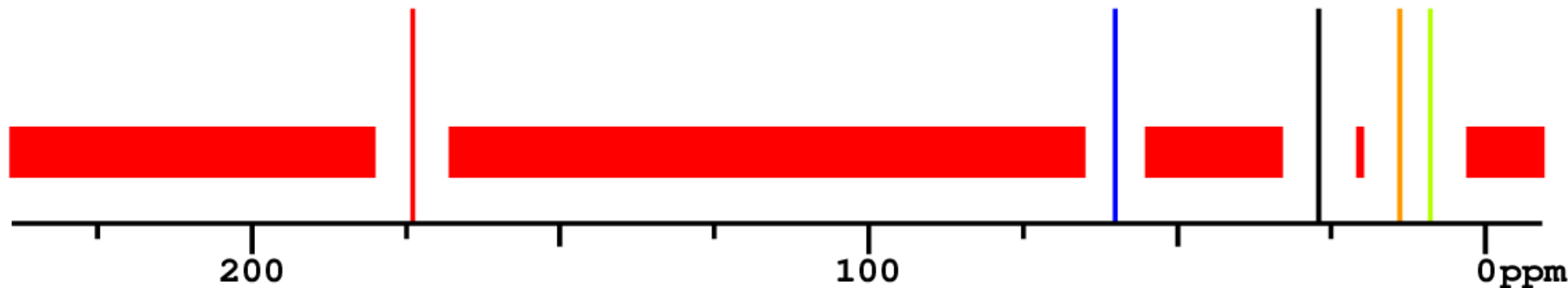
Predicted shift values

Signal multiplicity: S D T Q O E P ?



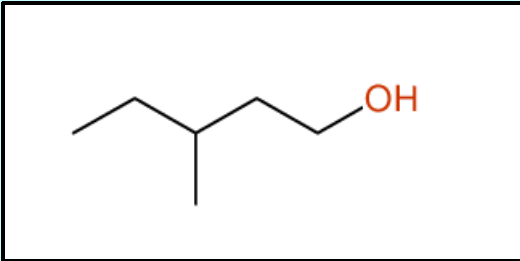
Experimental shift values

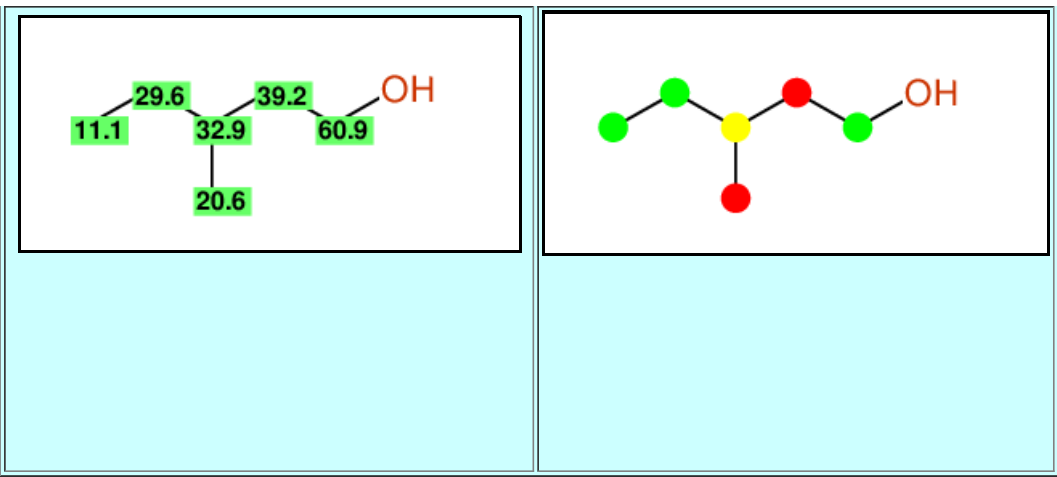
No line in reference: 



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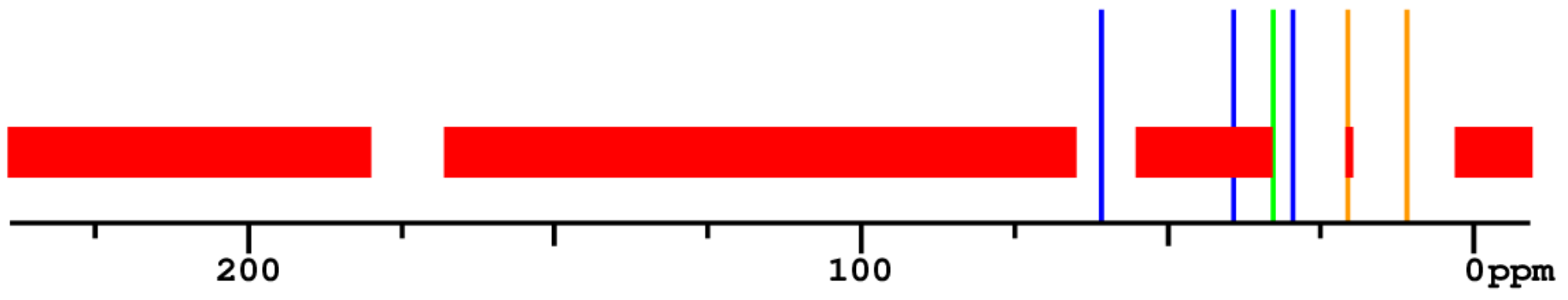
Structure Proposal #22

Structure	Similarity Measure
	<p>Deviation = 4.64 ppm Similarity = 58 % (Different pattern)</p> <p>$C_6H_{14}O$</p> <p>MWT = 102.07</p> <p>Search Web for this structure: IWTBVKIGCDZRPL</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



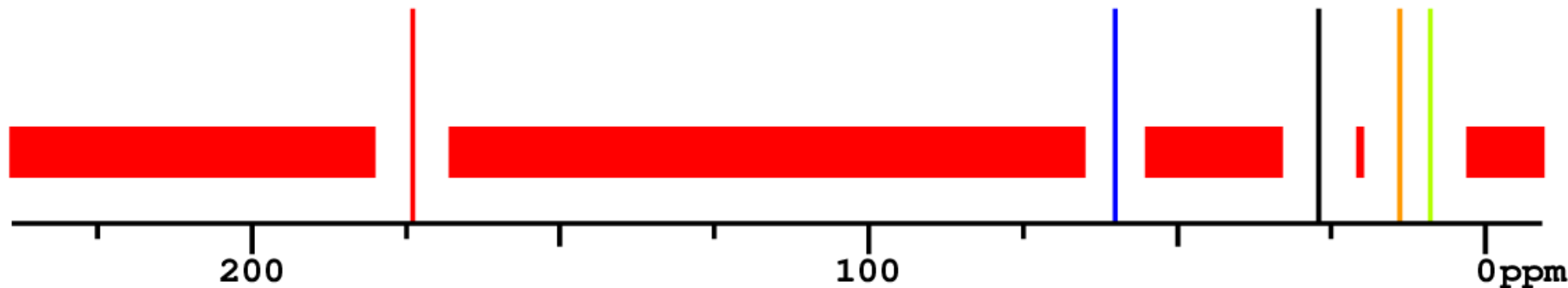
Predicted shift values

Signal multiplicity: S D T Q O E P ?



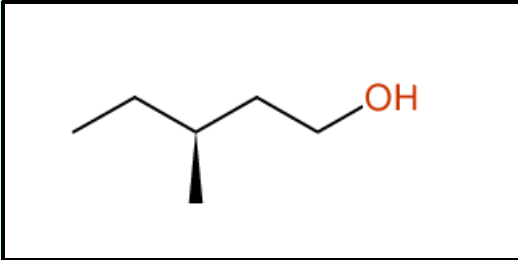
Experimental shift values

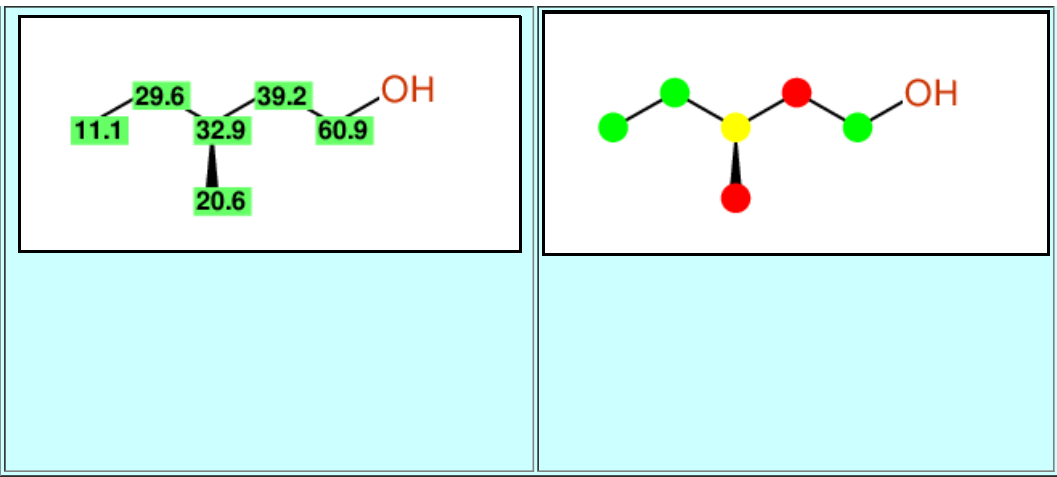
No line in reference: 



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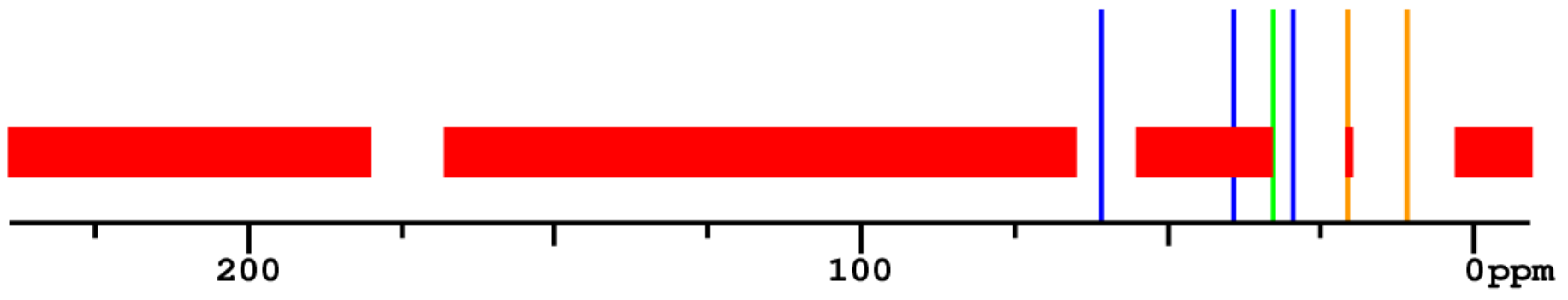
Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 4.64 ppm Similarity = 58 % (Different pattern)</p> <p>$C_6H_{14}O$</p> <p>MWT = 102.07</p> <p>Search Web for this structure: IWTVKIGCDZRPL</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



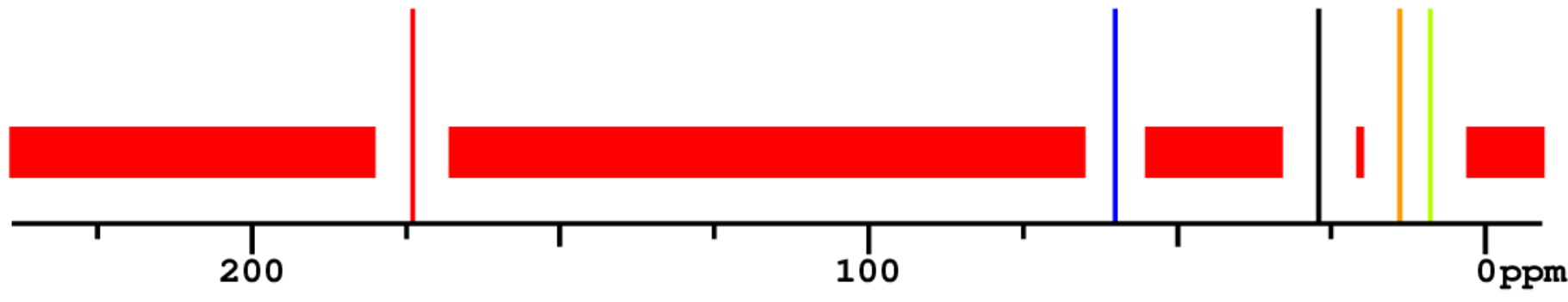
Predicted shift values

Signal multiplicity: S D T Q O E P ?



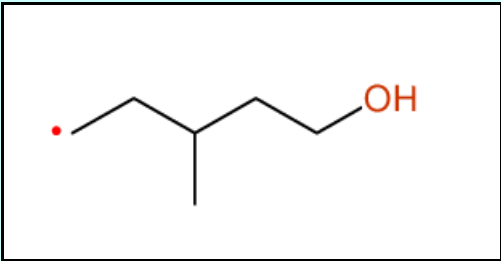
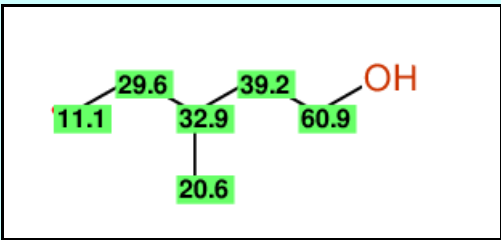
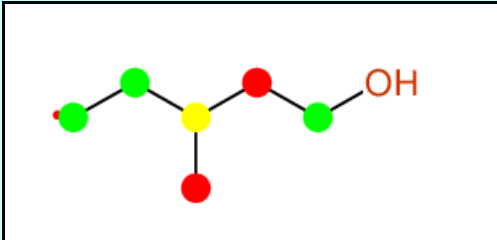
Experimental shift values

No line in reference: 



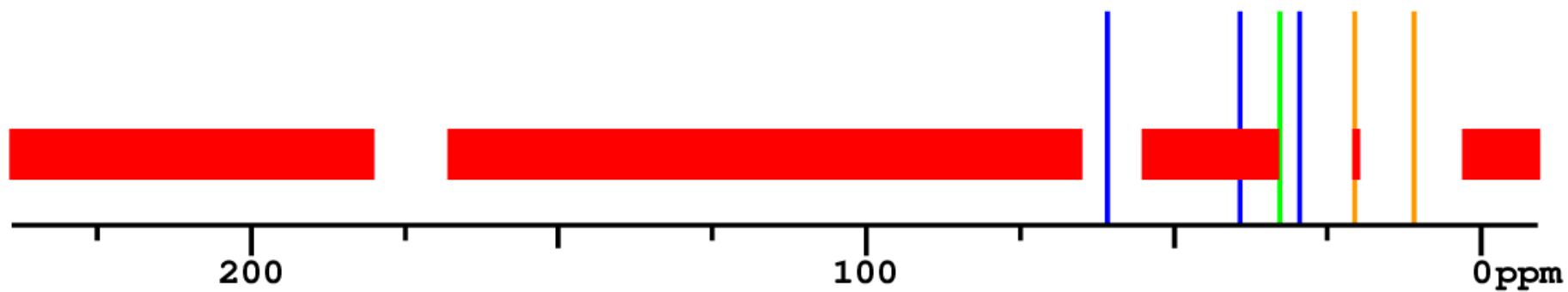
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Structure Proposal #24

Structure	Similarity Measure
	Deviation = 4.64 ppm Similarity = 58 % (Different pattern) $C_6H_{13}O$ MWT = 101.07 Search Web for this structure: FCACGIMTGMLTKJ
Predicted Chemical Shiftvalues	Matching Map
	

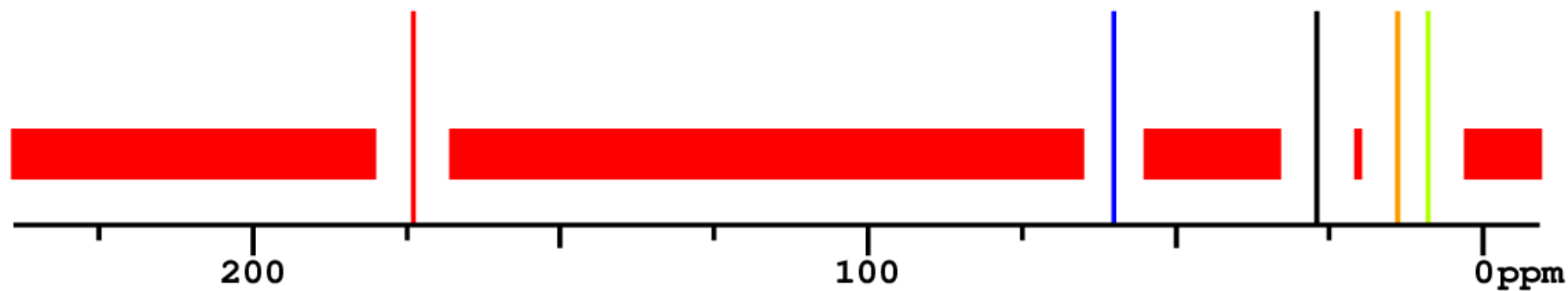
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

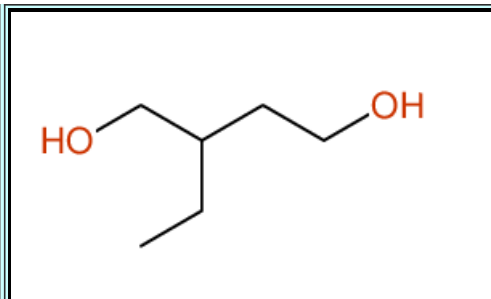
No line in reference: [red bar]



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Structure Proposal #25

Structure	Similarity Measure



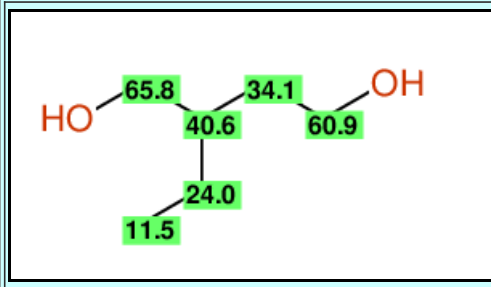
Deviation = 4.98 ppm
 Similarity = 50 %
 (Different pattern)

$C_6H_{14}O_2$

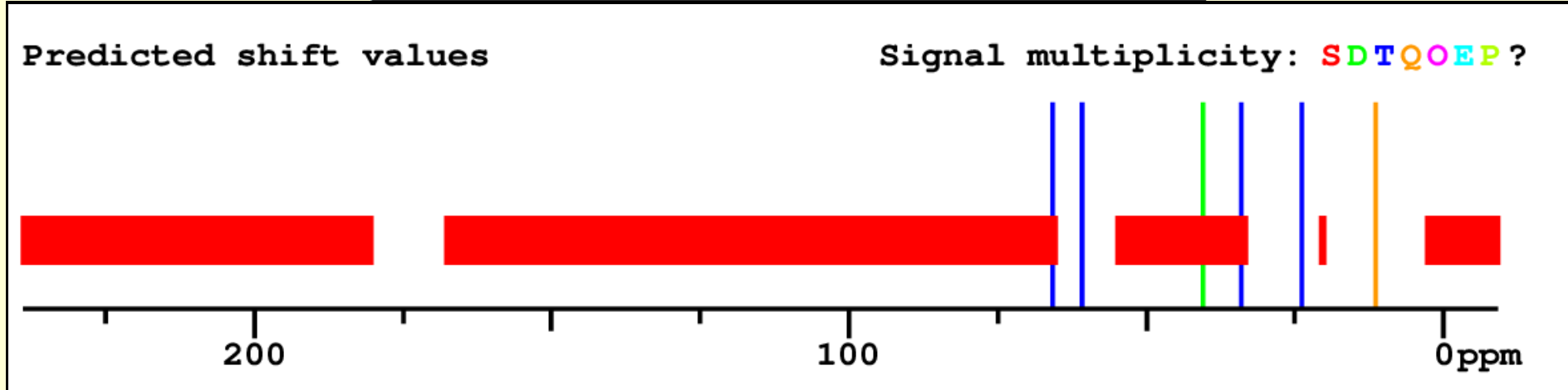
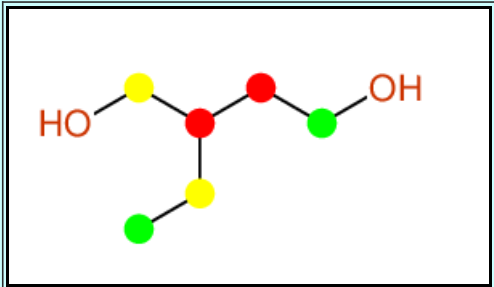
MWT = 118.07

Search Web for this structure:
[CYVMBANVYOZFIG](#)

Predicted Chemical Shiftvalues

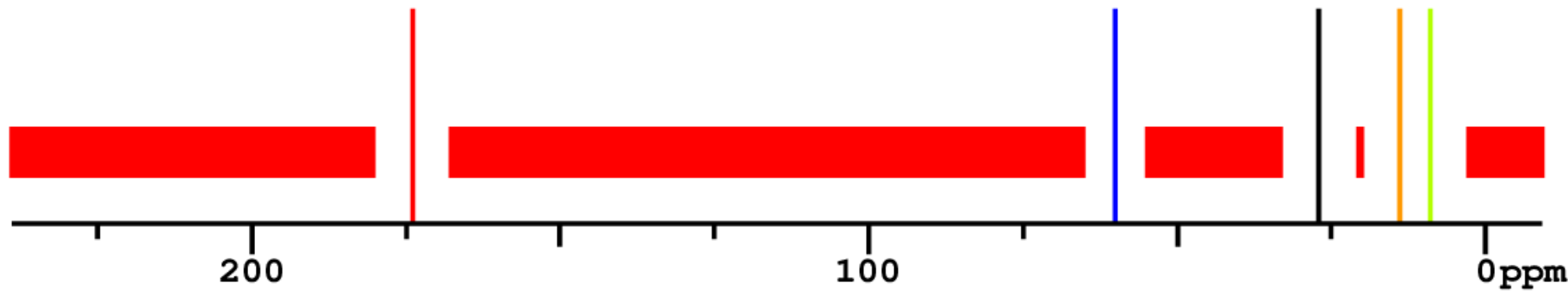


Matching Map



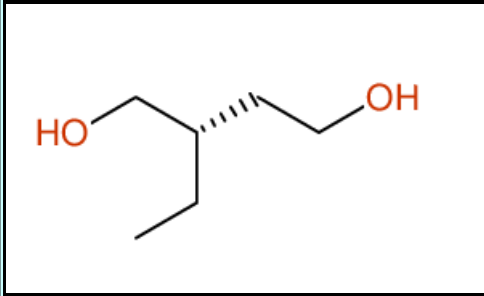
Experimental shift values

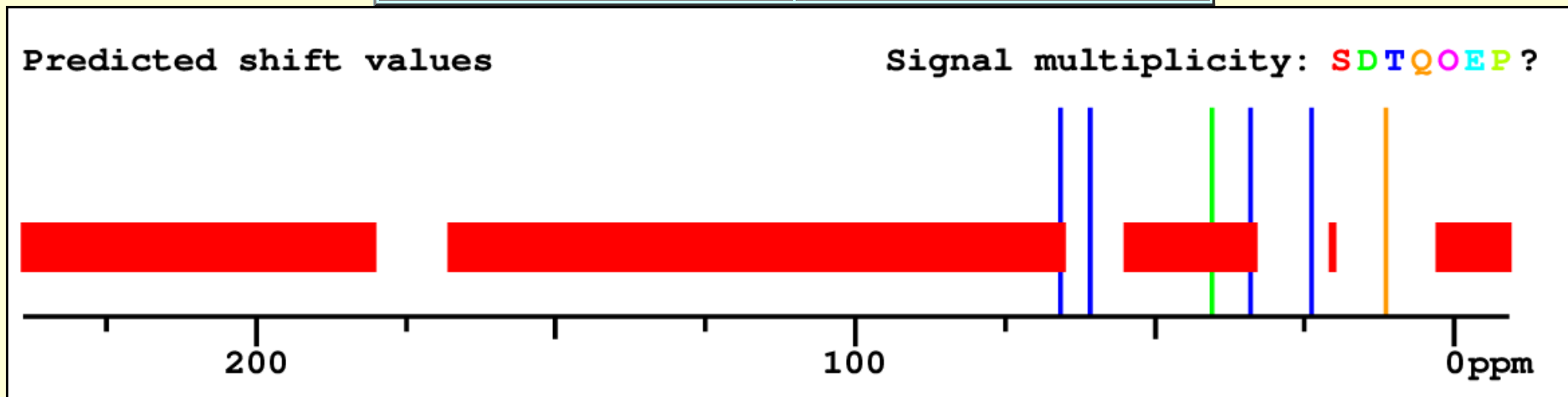
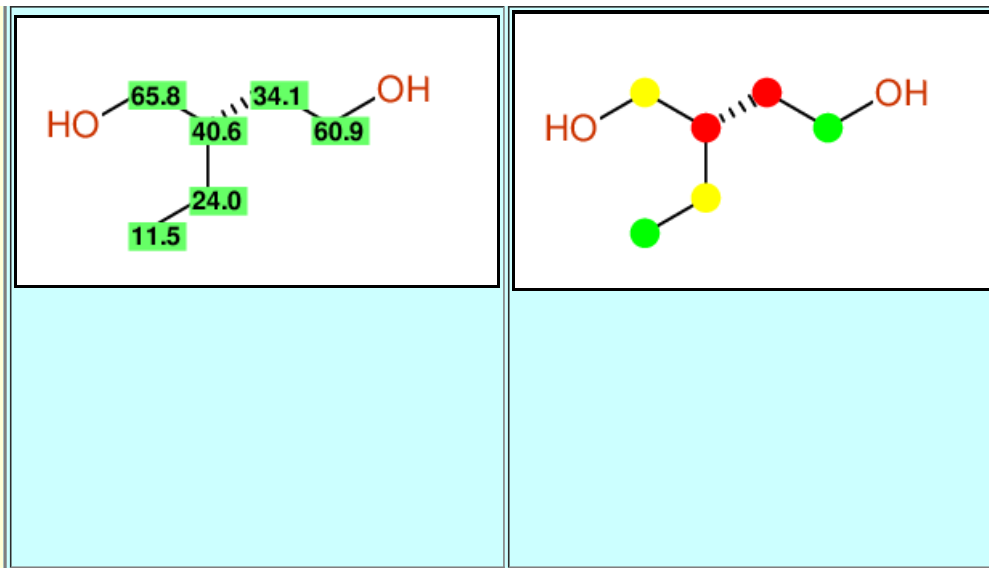
No line in reference: ██████████



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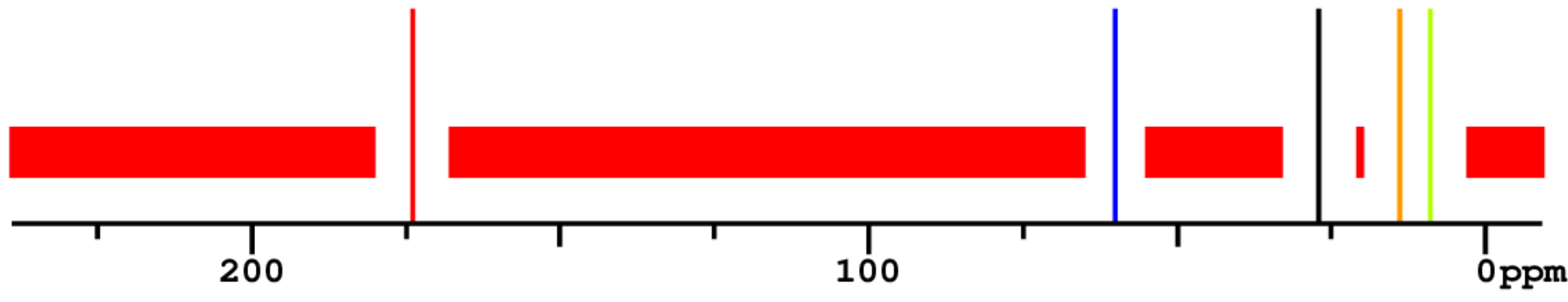
Structure Proposal #26

Structure	Similarity Measure
	<p>Deviation = 4.98 ppm Similarity = 50 % (Different pattern)</p> <p>$C_6H_{14}O_2$</p> <p>MWT = 118.07</p> <p>Search Web for this structure: CYVMBANVYOZFIG</p>
Predicted Chemical Shiftvalues	Matching Map



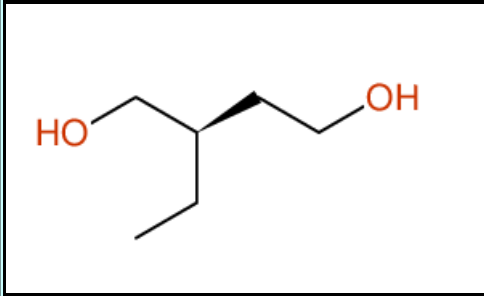
Experimental shift values

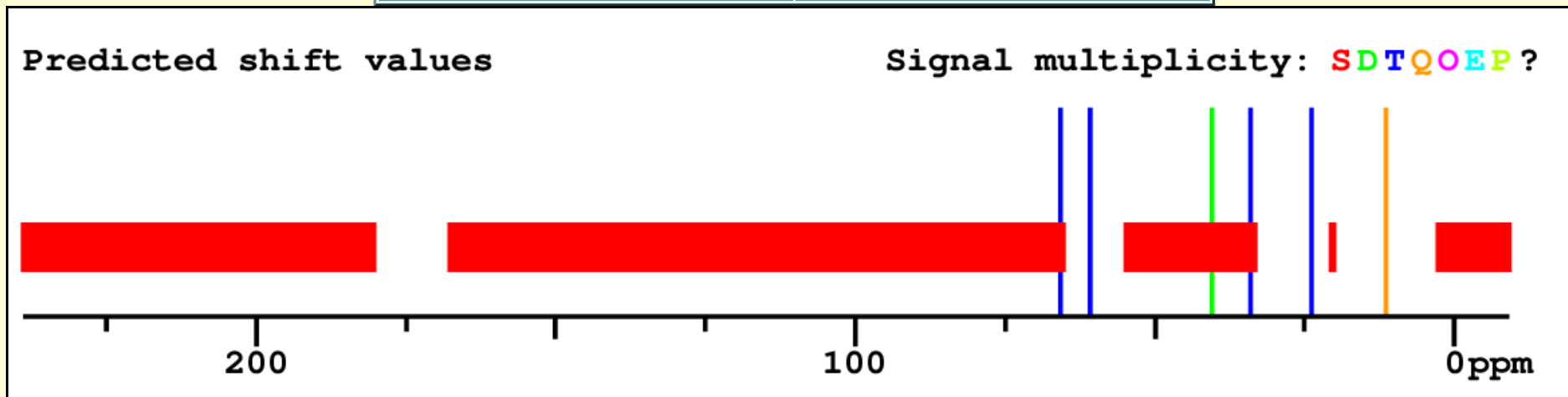
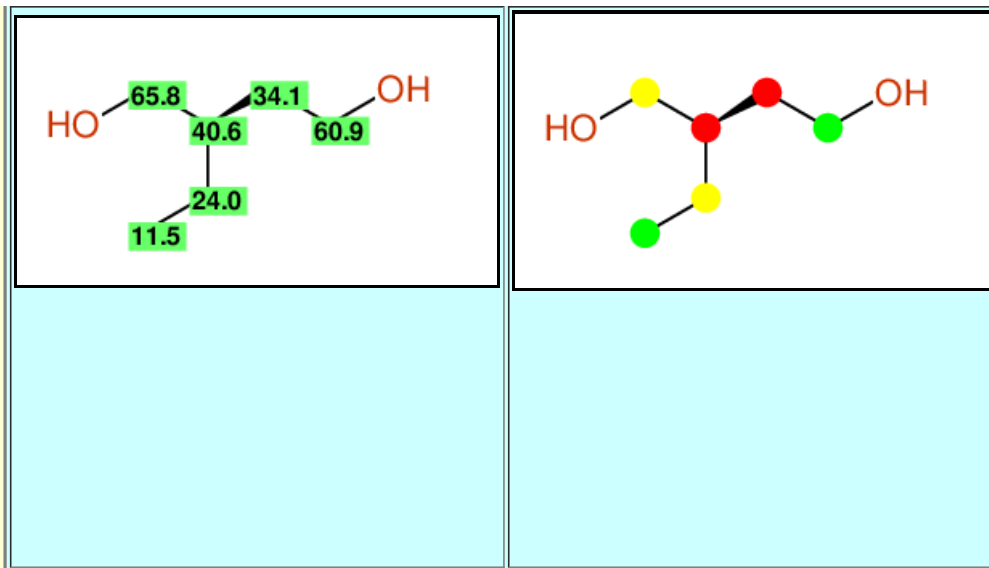
No line in reference: ████████



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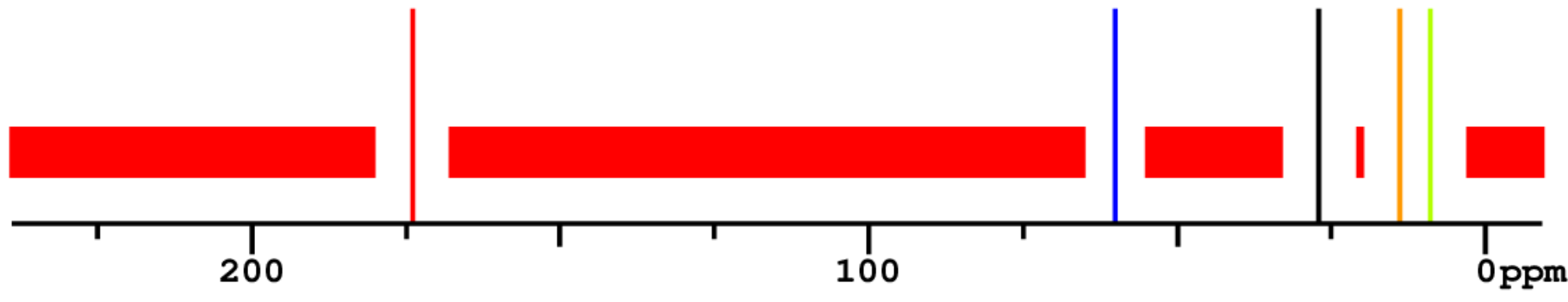
Structure Proposal #27

Structure	Similarity Measure
	<p>Deviation = 4.98 ppm Similarity = 50 % (Different pattern)</p> <p>$C_6H_{14}O_2$</p> <p>MWT = 118.07</p> <p>Search Web for this structure: CYVMBANVYOZFIG</p>
Predicted Chemical Shiftvalues	Matching Map



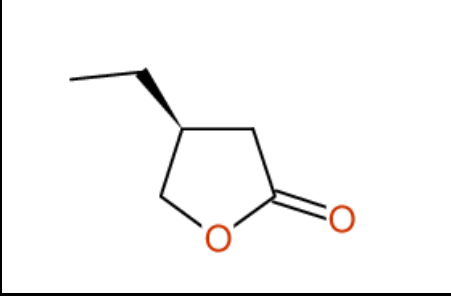
Experimental shift values

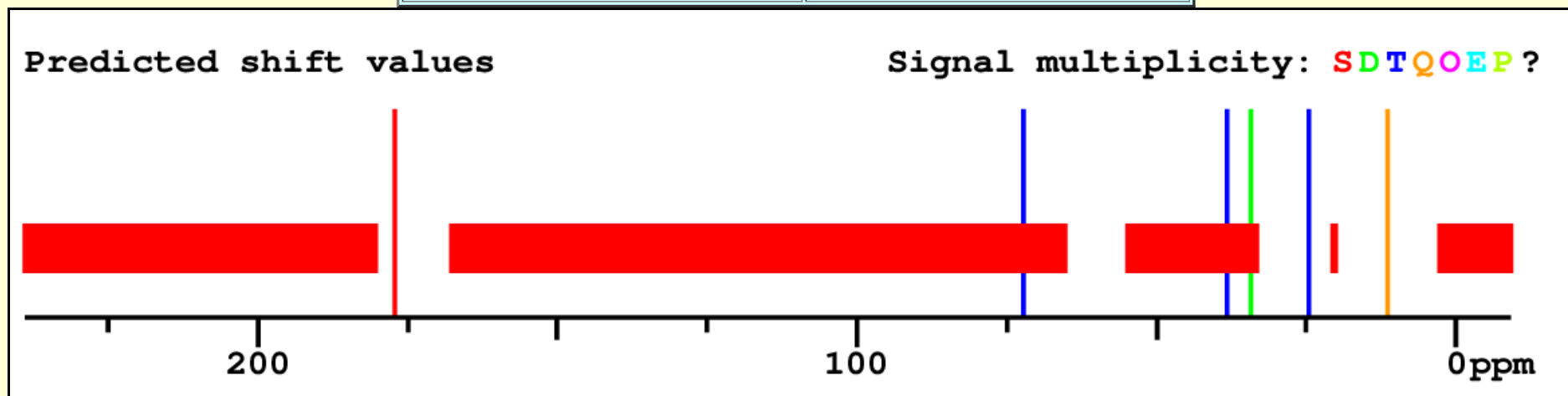
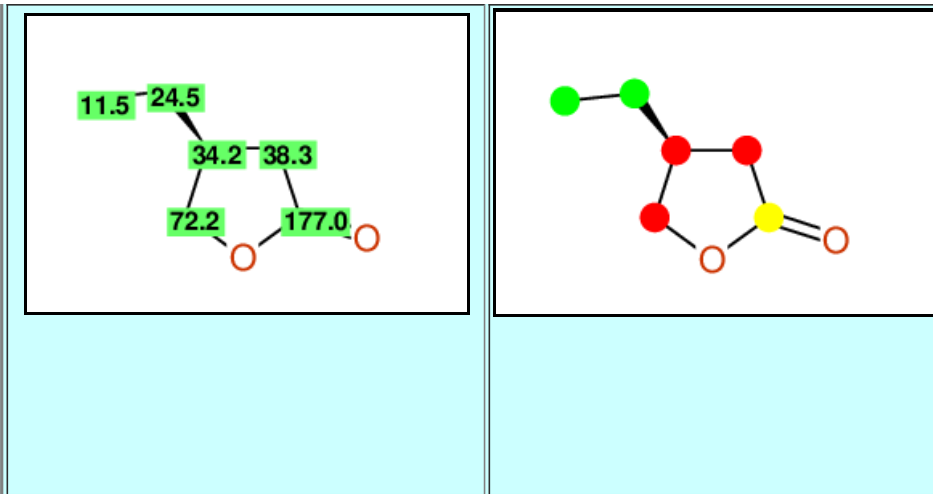
No line in reference: ████████

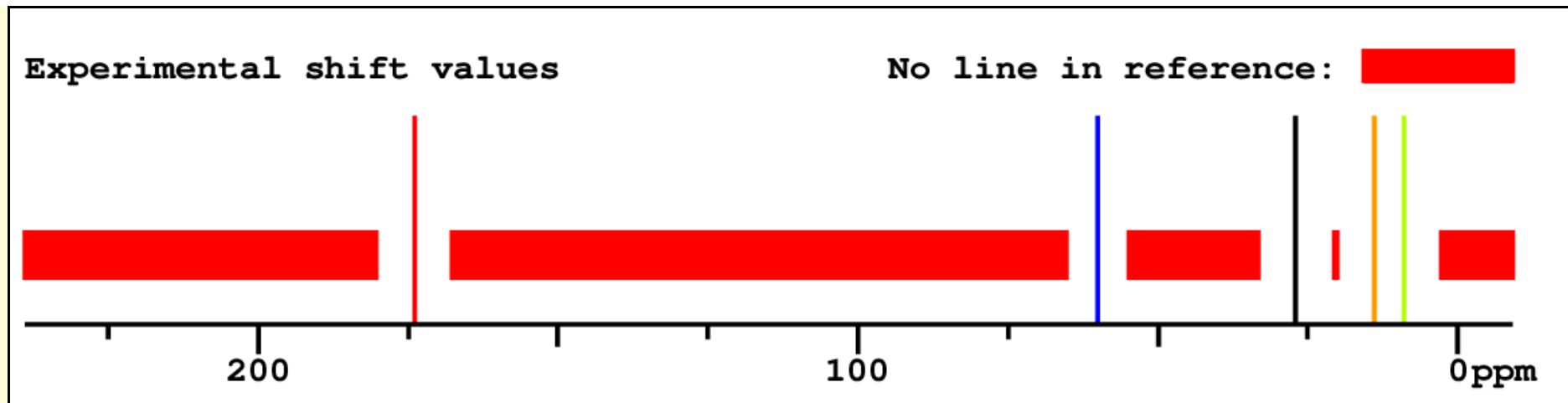


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Structure Proposal #28

Structure	Similarity Measure
	<p>Deviation = 6.77 ppm Similarity = 42 % (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>Search Web for this structure: MDQZVJSUBKPTHG</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map





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

<p>Occurence: 3 in 27</p>			
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Summary of Processing

Checking existence of data and counting them:	107,426,223 entries in 1.831 seconds
Applying restraints from elemental composition:	7.864 seconds, 3,176,524 entries remain

Applying restraints from number of signals:	2.866 seconds, 222,114 entries remain
Searching 1,956,285,417 chemical shift values line-per-line:	18.699 seconds
Best 1,528 entries selected for analysis:	2.686 seconds
Ranking of 1,528 entries by similarity:	73.021 seconds
Deviation of best match:	0.87 ppm
Creating table and linking 1,528 structures to 475,803 INCHIKEY-pages:	1.473 seconds
Detailed Analysis of 28 structures including graphical representation:	10.721 seconds
Analysis of 27 structures for common parent ring systems:	0.003 seconds
Total CPU-usage:	119.440 seconds
Data transferred from disk:	1,504 MBytes out of 1,695,823 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 19:12</p> <p>Have a nice day !</p>	