

Spectral Similarity Search based on
144,833,798 Structures
downloadable from the INTERNET
using CSEARCH - Technology

Description of Request

Please cite this service as:

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

Automatic Resubmit:

Multiplicity omitted

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:09

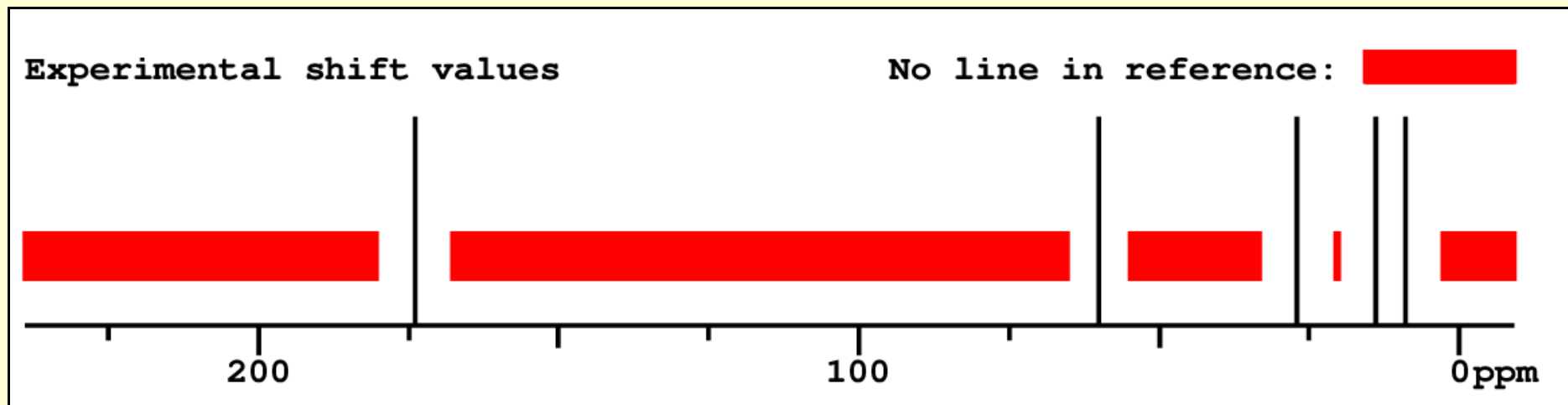
This page will be kept for 30 days here

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

Summary of Supplied Data

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

4	14.00	?	C or CH or CH ₂ or CH ₃	3.00
5	9.00	?	C or CH or CH ₂ or CH ₃	3.00



Additional Constraints given	
Any range more than 2*deviation (ppm) away from a query shiftvalue remains without line(s) in reference compounds	
Minimum number of signals in reference compounds:	3
Maximum number of signals in reference compounds:	7
Constraint from molecular weight already applied during search	

Lower limit for molecular weight:	85.00
Upper limit for molecular weight:	120.00
N	Element must be absent
O	Element must be present
P	Element must be absent
S	Element must be absent
F	Element must be absent
Cl	Element must be absent
Br	Element must be absent
I	Element must be absent
other	Element must be absent

Elemental Composition of Reference Structures

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

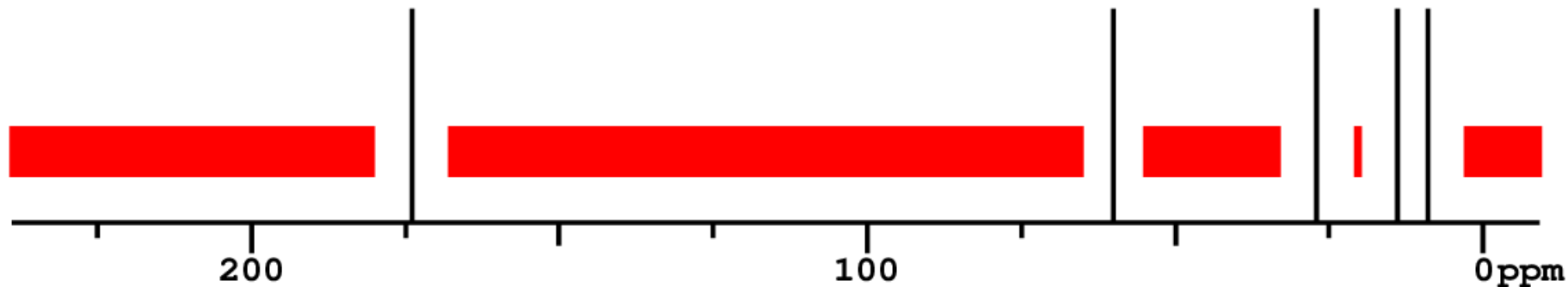
Available entries at each Screening-Step

Total number of entries:	144,833,798
Applying requested elemental composition:	3,593,931 entries remain
Applying requested number of signals:	104,807 entries remain

Entries per line found out of 104,807 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	?	3.00	12,167	Impurity ?
2	60.00	?	2.50	18,863	Unspecific line
3	27.00	?	3.00	39,616	Unspecific line
4	14.00	?	3.00	26,162	Unspecific line
5	9.00	?	3.00	18,435	Unspecific line

Experimental shift values

No line in reference: 



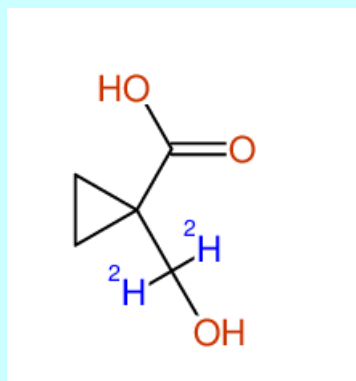
Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	38	Selected for detailed analysis
4	852	Selected for detailed analysis
3	6,458	Selected for detailed analysis
2	24,043	
1	44,185	

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

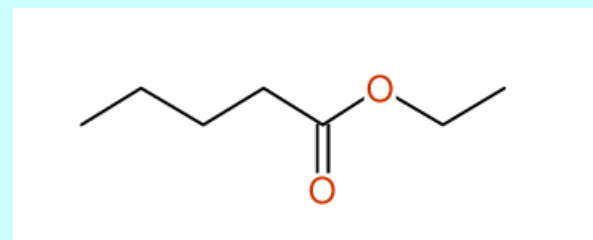
2.21 -
2.21ppm

1x found [TYFMINBPAYVYCW](#)



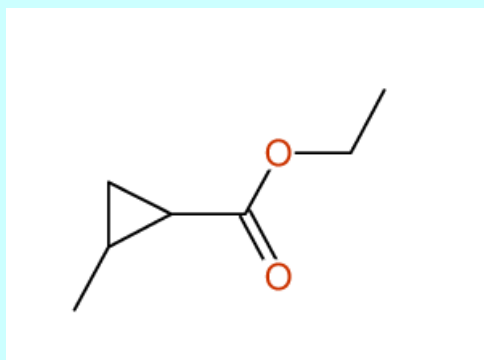
2.73 -
2.73ppm

1x found [VUXQCEFKOQUTQO](#)



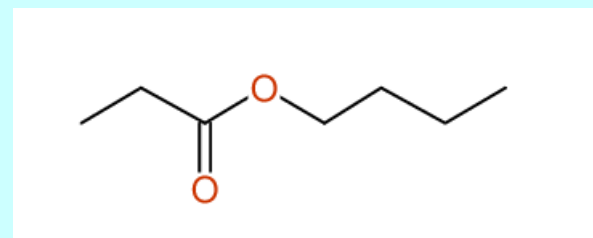
2.77 -
2.77ppm

1x found [ZNXRPIKPYJZPNI](#)



2.96 -
2.96ppm

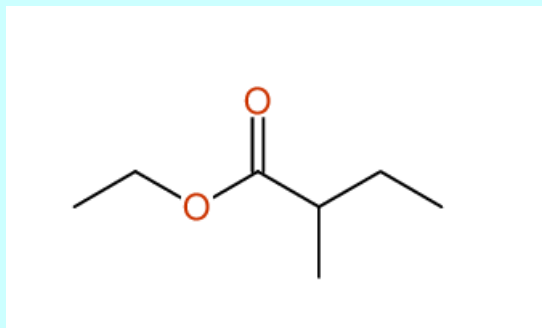
1x found [YQKXIRZLKBWITR](#)



3.41 -
3.41ppm

1x found

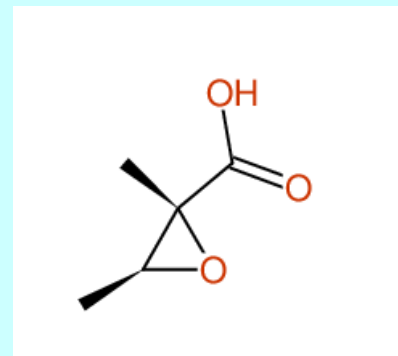
[JPVJJBICKBKSH](#)



3.54 -
3.54ppm

1x found

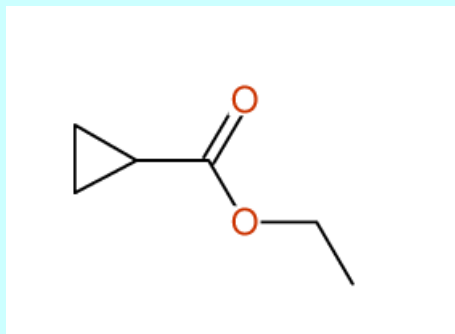
[RUFMEDUWOSHOHF](#)



3.54 -
3.54ppm

1x found

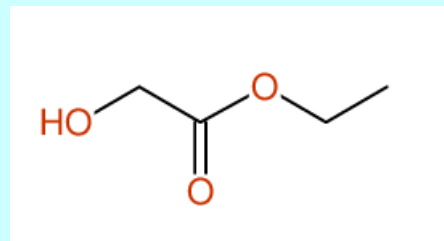
[OARDGAWFHAUOJC](#)



3.72 -
3.72ppm

1x found

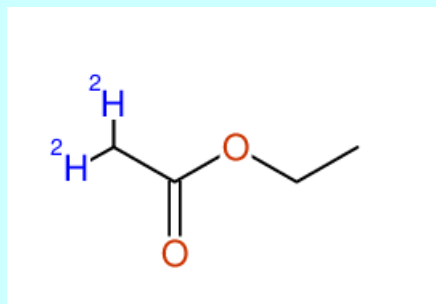
[USTOPXSKJLOMG](#)



3.74 -
3.74ppm

1x found

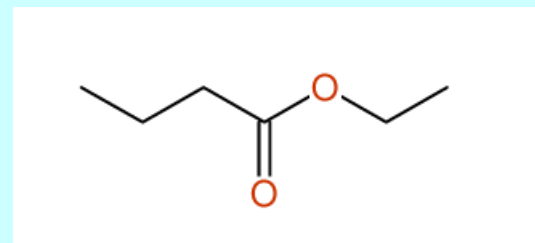
[XEKOWRVHYACXOJ](#)



4.02 -
4.02ppm

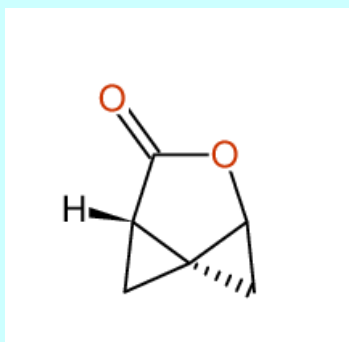
1x found

[OBNCKNCVKJNDBV](#)



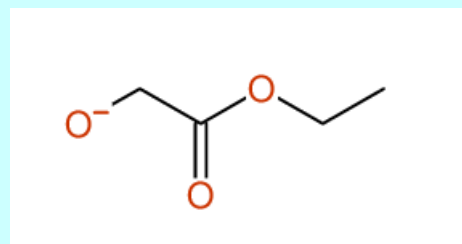
4.04 -
4.04ppm

1x found [WZLNCRVWIKHJER](#)



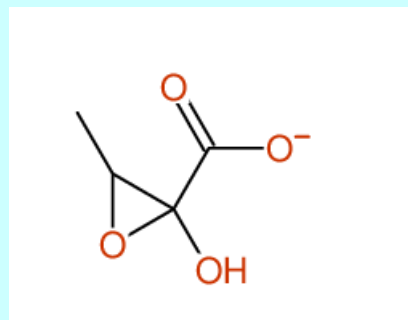
4.11 -
4.11ppm

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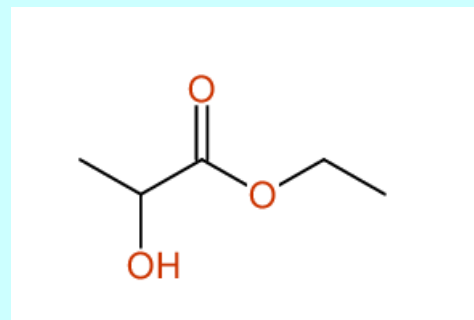
4.23 -
4.23ppm

1x found [KYFIXARGJXDBJJ](#)



4.33 -
4.33ppm

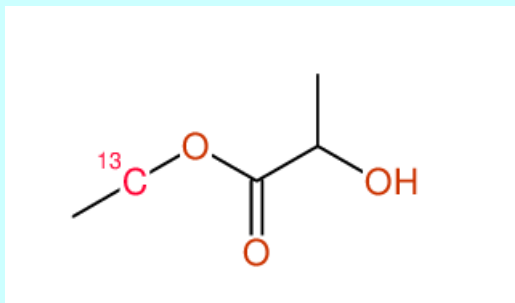
1x found [FPXAEZNSBIIYFJ](#)



4.33 -
4.33ppm

1x found

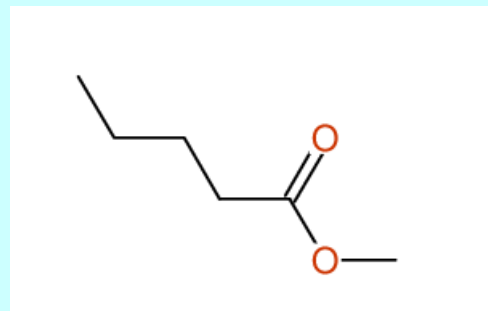
[LZCLXQDLBQLTDK](#)



4.57 -
4.57ppm

1x found

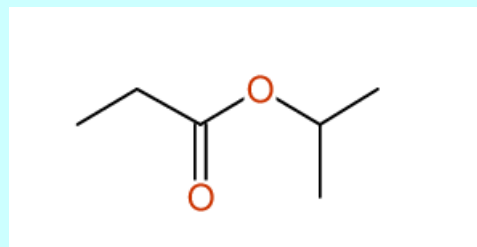
[MHBOACTUGJRRKE](#)



4.65 -
4.65ppm

1x found

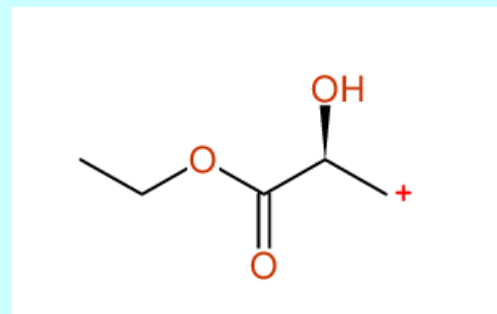
[IMNXURKAQGHYAH](#)



4.70 -
4.70ppm

2x found

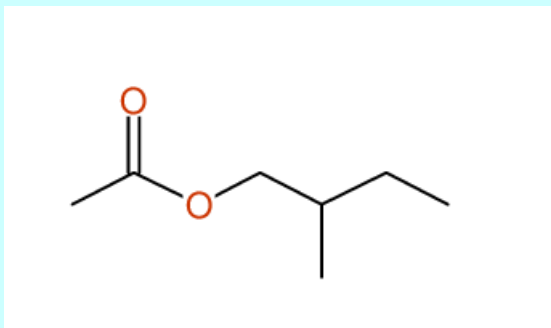
[SFMRLHJNHWEFDX](#)



4.75 -
4.75ppm

1x found

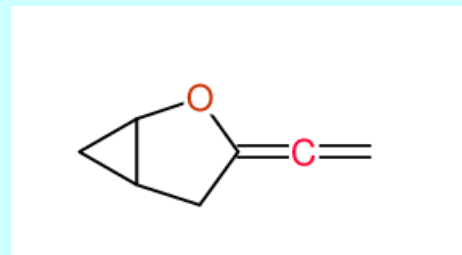
[APXBKUAJSWJTRL](#)



5.23 -
5.23ppm

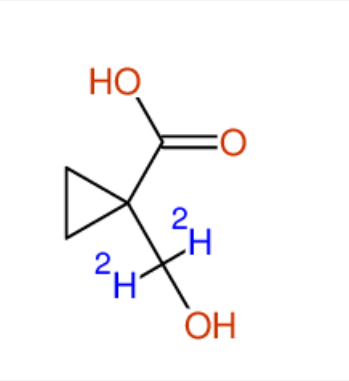
1x found

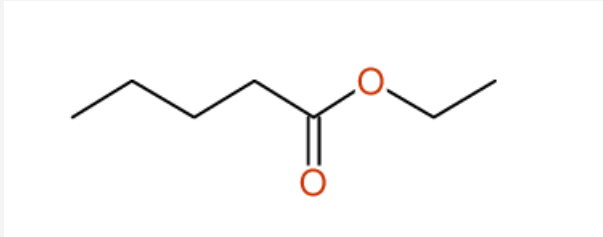
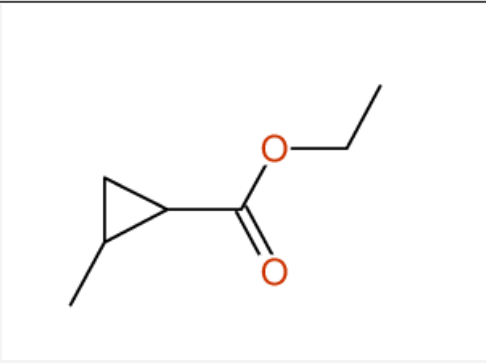
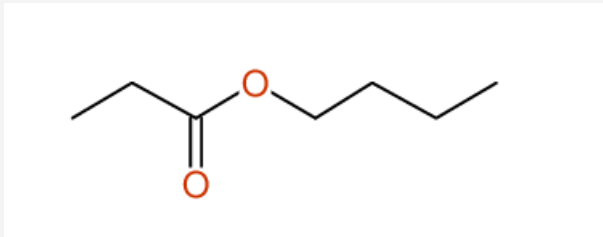
[HPLLJBRTSULDDV](#)

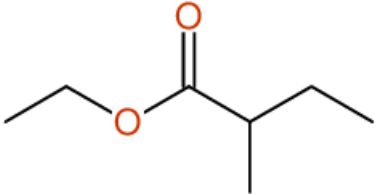
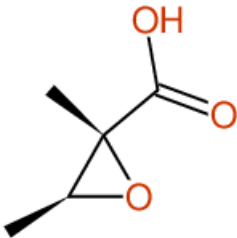
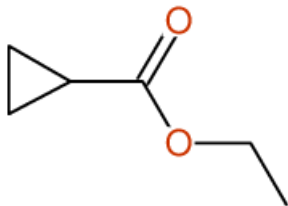
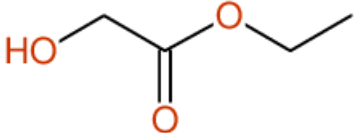


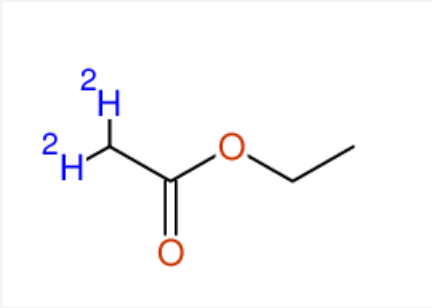

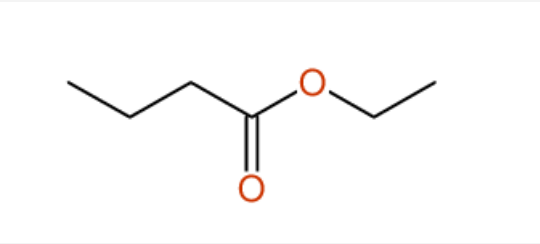

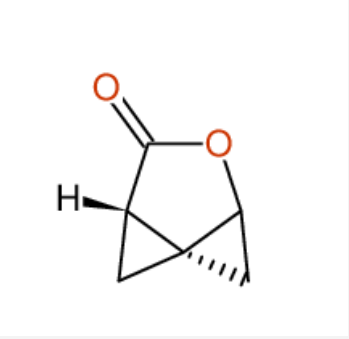
7,348 [Structure proposals](#) found for your C-NMR Spectrum

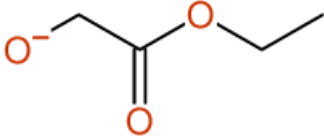
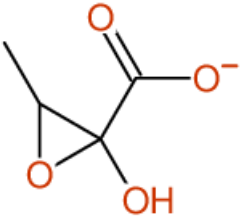
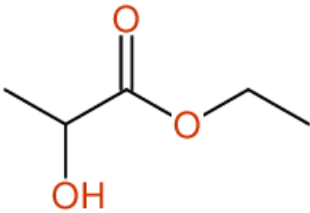
375 Entries will be shown because of your selection of additional constraints

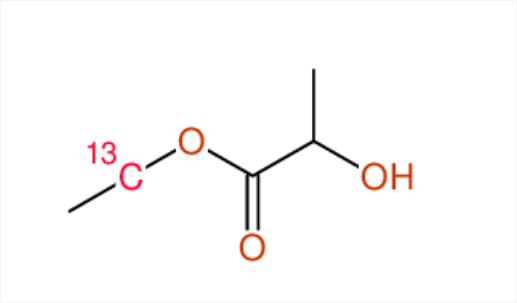

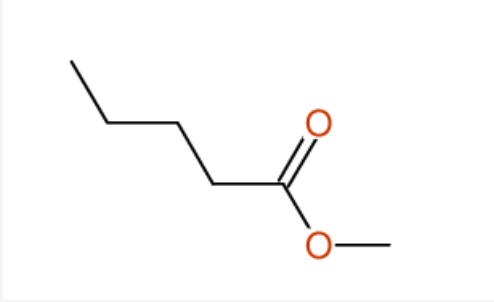
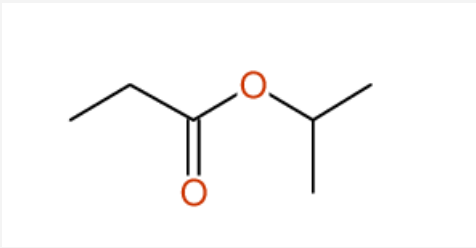
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1 2.21 Details	 <p>Chemical structure of 1,1-dihydroxycyclopropane-2-carboxylic acid, showing a cyclopropane ring with two hydroxyl groups on one carbon and a carboxylic acid group on an adjacent carbon.</p>	C ₅ H ₈ O ₃ MWT = 118.055	Proposal #1 Structure-ID: 36,333,767 TYFMINBPAYVYCW-SMZGMGDZEE	

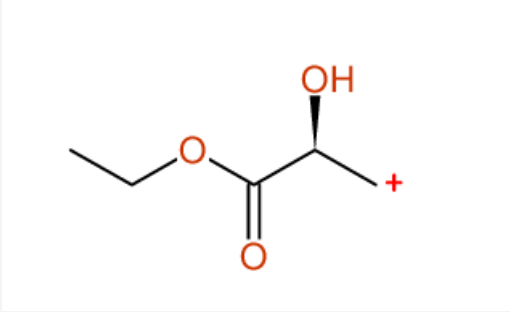
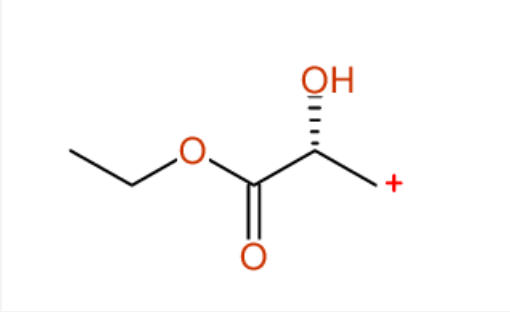
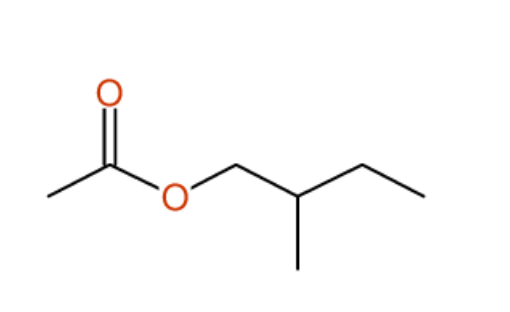
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #2 2.73 Details Different pattern		C_7O_2 MWT = 116.077	Proposal #2 Structure-ID: 143,973,553 VUXQCEFKOQUTQO-UHFFFAOYAP	
Proposal #3 2.77 Details		C_7O_2 MWT = 116.077	Proposal #3 Structure-ID: 143,974,183 ZNXRPIKPYJZPNI-UHFFFAOYAZ	
Proposal #4 2.96 Details Different pattern		C_7O_2 MWT = 116.077	Proposal #4 Structure-ID: 143,961,843 YQKXIRZLKBWITR-UHFFFAOYAA	

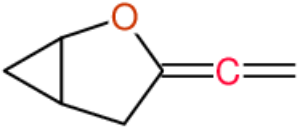
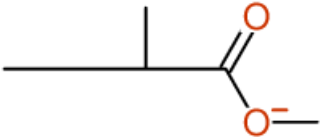
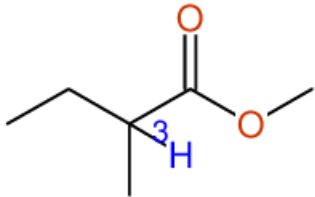

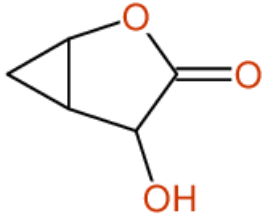
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #5 3.41 Details Different pattern		C_7O_2 MWT = 116.077	Proposal #5 Structure-ID: 106,480,336 JPVJIJBICKBKSH-UHFFFAOYAB	
Proposal #6 3.54 Details Different pattern		C_5O_3 MWT = 108.055	Proposal #6 Structure-ID: 144,050,371 RUFMEDUWOSHOHF-RXMQYKEDBN	
Proposal #7 3.54 Details		C_6O_2 MWT = 104.066	Proposal #7 Structure-ID: 143,974,802 OARDGAWFHUAUJC-UHFFFAOYAC	
Proposal #8 3.72 Details		C_4O_3 MWT = 96.044	Proposal #8 Structure-ID: 143,973,744 USTOPXSKJLOMKG-UHFFFAOYAE	

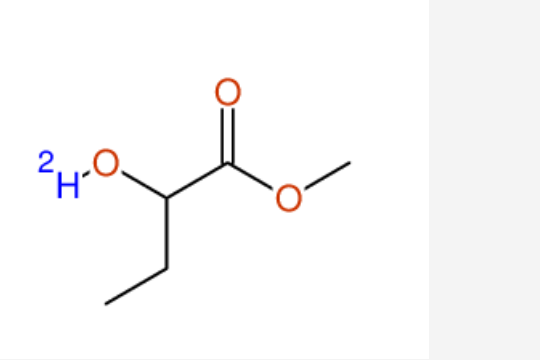
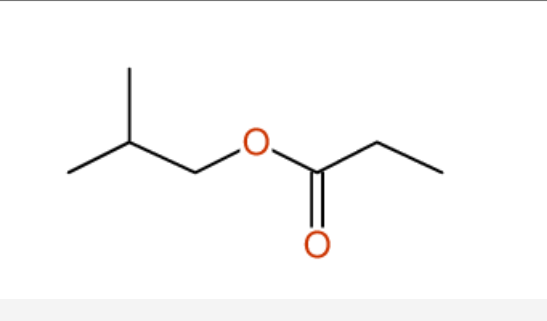
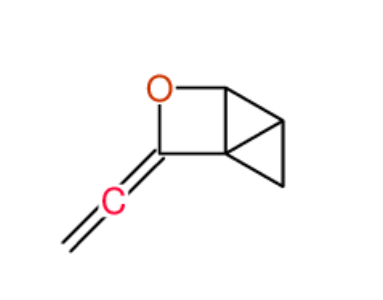
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #9</p> <p>3.74</p> <p>Details</p> <p>Different pattern</p>		<p>$C_4H_8O_2$</p> <p>MWT = 90.044</p>	<p>Proposal #9</p> <p>Structure-ID: 92,737,183</p> <p>XEKOWRVHYACXOJ-CBTSVUPCEF</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #10</p> <p>4.02</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{12}O_2$</p> <p>MWT = 116.066</p>	<p>Proposal #10</p> <p>Structure-ID: 135,913,890</p> <p>OBNCKNCVKJNDBV-IKLDfBCSAI</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #11</p> <p>4.04</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_6O_2$</p> <p>MWT = 110.066</p>	<p>Proposal #11</p> <p>Structure-ID: 95,068,850</p> <p>WZLNCRVWIKHJER-RSJRKSSKBF</p>	

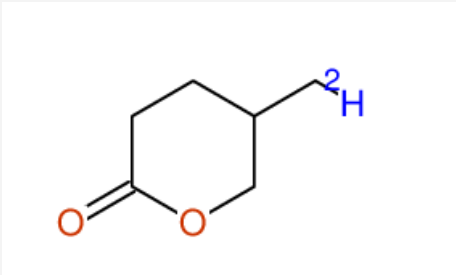

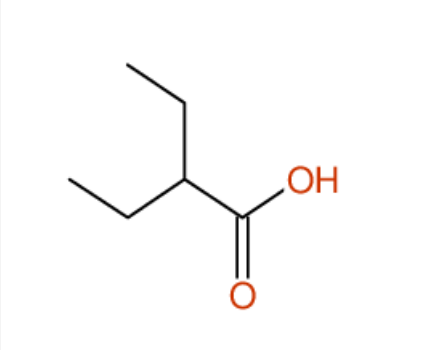
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #12 4.11 Details		$C_4H_7O_2$ MWT = 103.044	Proposal #12 Structure-ID: 98,518,941 PDHCCQJYEKLVRY-UHFFFAOYAC	
Proposal #13 4.23 Details		$C_5H_8O_4$ MWT = 118.044	Proposal #13 Structure-ID: 97,391,778 KYFIXARGJXDBJJ-REWHXWOFAM	
Proposal #14 4.33 Details Different pattern		$C_7H_{14}O_3$ MWT = 130.095	Proposal #14 Structure-ID: 106,386,754 FPXAEZNSBIIFJ-UHFFFAOYAT	

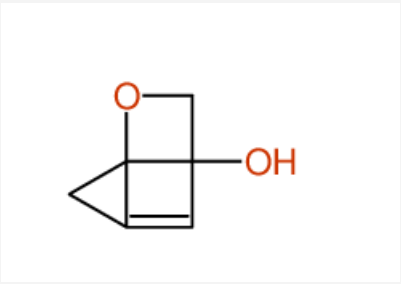
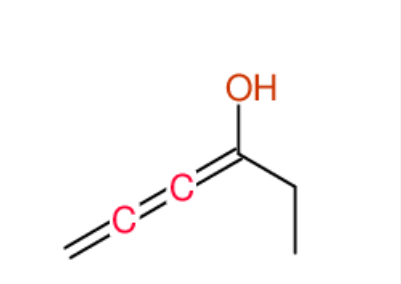
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #15 4.33 Details Different pattern		$C_5H_{10}O_3$ MWT = 119.055	Proposal #15 Structure-ID: 91,226,937 LZCLXQDLBQLTDK-LBPDFUHNES	Availability of NMR-Data in CSEARCH 
Proposal #16 4.57 Details Different pattern		C_6O_2 MWT = 104.066	Proposal #16 Structure-ID: 106,387,374 MHBOACTUGJRRKF-UHFFFAOYAS	
Proposal #17 4.65 Details Different pattern		C_6O_2 MWT = 104.066	Proposal #17 Structure-ID: 106,489,994 IMNXURKAQGHYAH-UHFFFAOYAM	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #18</p> <p>4.70</p> <p>Details</p>		<p>C₅H₉O₃</p> <p>MWT = 117.055</p>	<p>Proposal #18</p> <p>Structure-ID: 90,719,745</p> <p>SFMLRHJNHWEFDX-BYPYZUCNBM</p>	
<p>Proposal #19</p> <p>4.70</p> <p>Details</p>		<p>C₅H₉O₃</p> <p>MWT = 117.055</p>	<p>Proposal #19</p> <p>Structure-ID: 90,719,746</p> <p>SFMLRHJNHWEFDX-SCSAIBSYBB</p>	
<p>Proposal #20</p> <p>4.75</p> <p>Details</p> <p>Different pattern</p>		<p>C₇O₂</p> <p>MWT = 116.077</p>	<p>Proposal #20</p> <p>Structure-ID: 106,478,409</p> <p>APXBKUAJSWJTRL-UHFFFAOYAX</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #21 5.23 Details Different pattern		C_7H_8O MWT = 108.077	Proposal #21 Structure-ID: 61,877,050 HPLLJBRTSULDDV-UHFFFAOYAX	
Proposal #22 5.23 Details Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #22 Structure-ID: 11,897,837 DREXZGTZFACURF-UHFFFAOYAA	
Proposal #23 5.25 Details Different pattern		$C_6H_{12}O_2$ MWT = 118.066	Proposal #23 Structure-ID: 96,324,531 OCWLYWIFNDCWRZ-XHHURNKPEV	Availability of NMR-Data in CSEARCH 
Proposal #24 5.46 Details Different pattern		$C_5H_6O_3$ MWT = 114.055	Proposal #24 Structure-ID: 78,340,100 YYYNYNGRONAJGI-UHFFFAOYAI	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #25</p> <p>5.48</p> <p>Details</p> <p>Different pattern</p>		<p>$C_5H_{10}O_3$</p> <p>MWT = 119.055</p>	<p>Proposal #25</p> <p>Structure-ID: 18,031,616</p> <p>DDMCDMDOHABRHD-RAMDWTOOER</p>	
<p>Proposal #26</p> <p>5.66</p> <p>Details</p> <p>Different pattern</p>		<p>C_7O_2</p> <p>MWT = 116.077</p>	<p>Proposal #26</p> <p>Structure-ID: 106,489,920</p> <p>CPOGEOGDMOTURU-UHFFFAOYAN</p>	
<p>Proposal #27</p> <p>5.83</p> <p>Details</p>		<p>C_7H_6O</p> <p>MWT = 106.077</p>	<p>Proposal #27</p> <p>Structure-ID: 70,205,768</p> <p>DCKHOMFWTGMJOV-UHFFFAOYAX</p>	

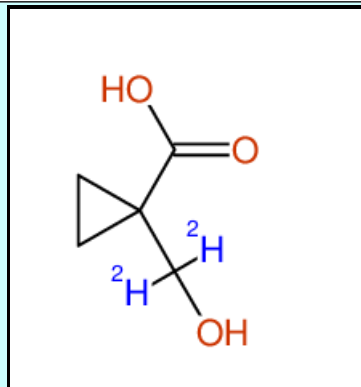
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #28</p> <p>5.85</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 115.066</p>	<p>Proposal #28</p> <p>Structure-ID: 99,656,932</p> <p>GQUBDAOKWZLWDI-MICDWDOJER</p>	<p>Availability of NMR-Data in CSEARCH</p> 
<p>Proposal #29</p> <p>5.96</p> <p>Details</p> <p>Different pattern</p>		<p>C_6O_2</p> <p>MWT = 104.066</p>	<p>Proposal #29</p> <p>Structure-ID: 106,467,443</p> <p>CUXRHJZMBXDZPJ-UHFFFAOYAC</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #30 6.89 Details Different pattern		C₆H₆O₂ MWT = 110.066	Proposal #30 Structure-ID: 78,918,450 INDSDELFJIPJJU-UHFFFAOYAU	
Proposal #31 6.91 Details Different pattern		C₆H₈O MWT = 96.066	Proposal #31 Structure-ID: 119,846,386 XFXVNBAJTJGVQJ-UHFFFAOYAG	

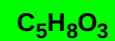
Detailed Analysis

Structure Proposal #1

Structure	Similarity Measure



Deviation = 2.21 ppm
Similarity = 100 %

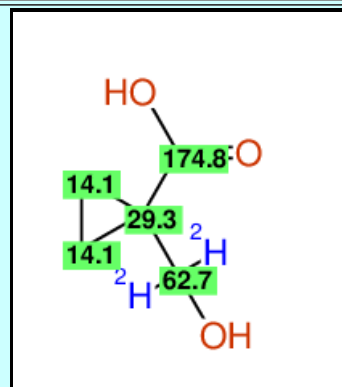


MWT = 118.06

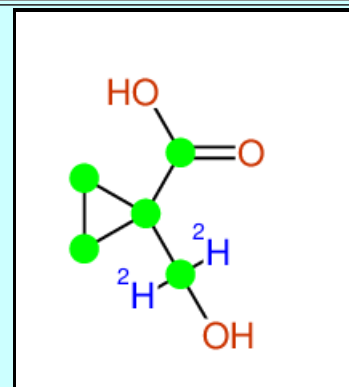
Search Web for this structure:

[TYEMINBPAYVCW](#)

Predicted Chemical Shiftvalues

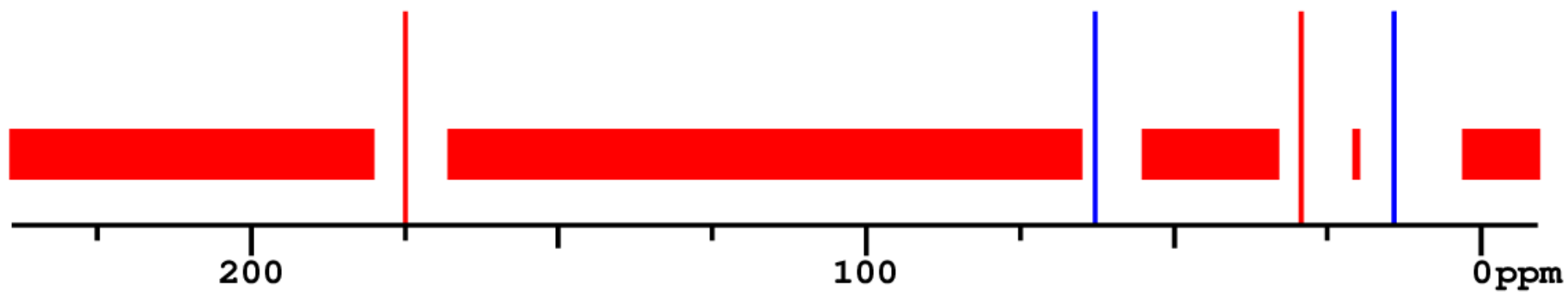


Matching Map



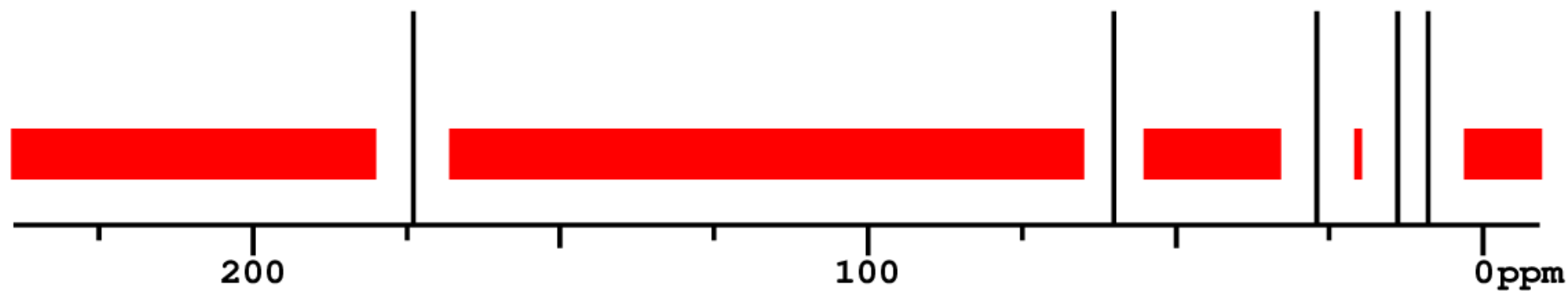
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

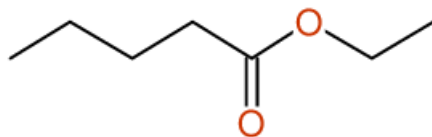
No line in reference: [red bar]



[Back to Complete Result](#)

Structure Proposal #2

Structure	Similarity Measure



Deviation = 2.73 ppm
 Similarity = 79 %
 (Different pattern)

C_7O_2

MWT = 116.08

Search Web for this structure:

[VUXQCEFKOQUTQO](#)

Predicted Chemical Shiftvalues

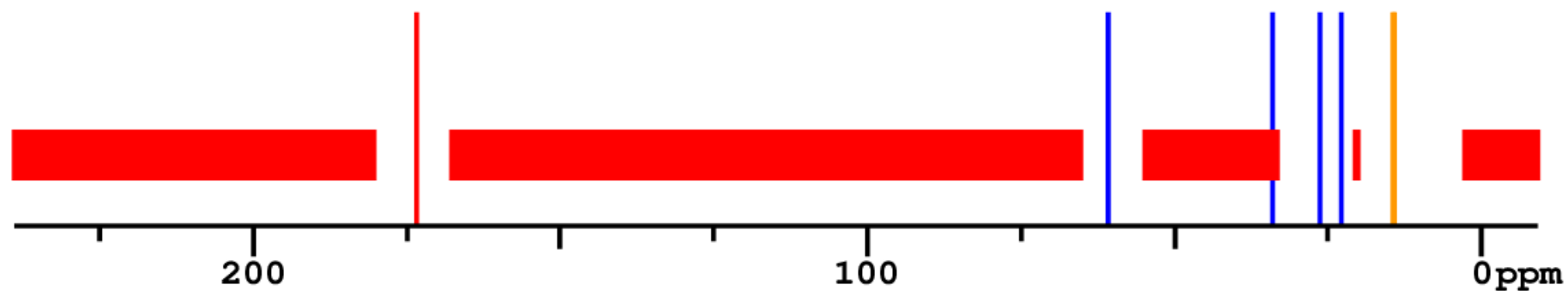


Matching Map



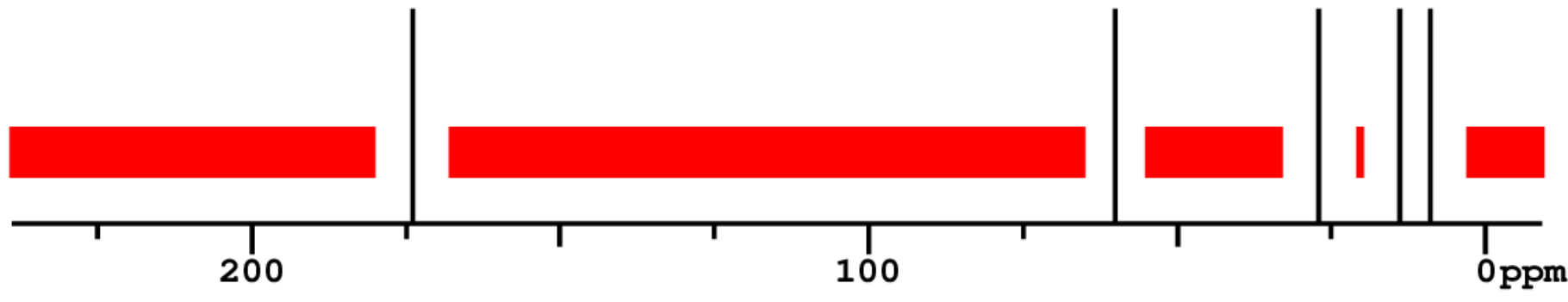
Predicted shift values

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



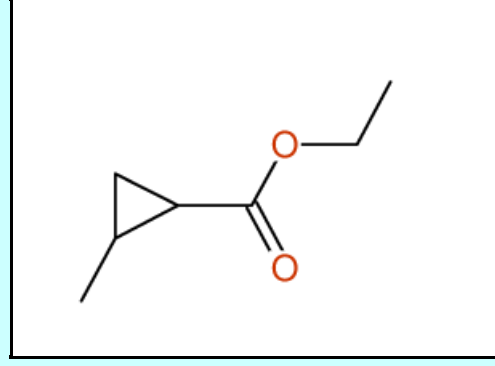
Experimental shift values

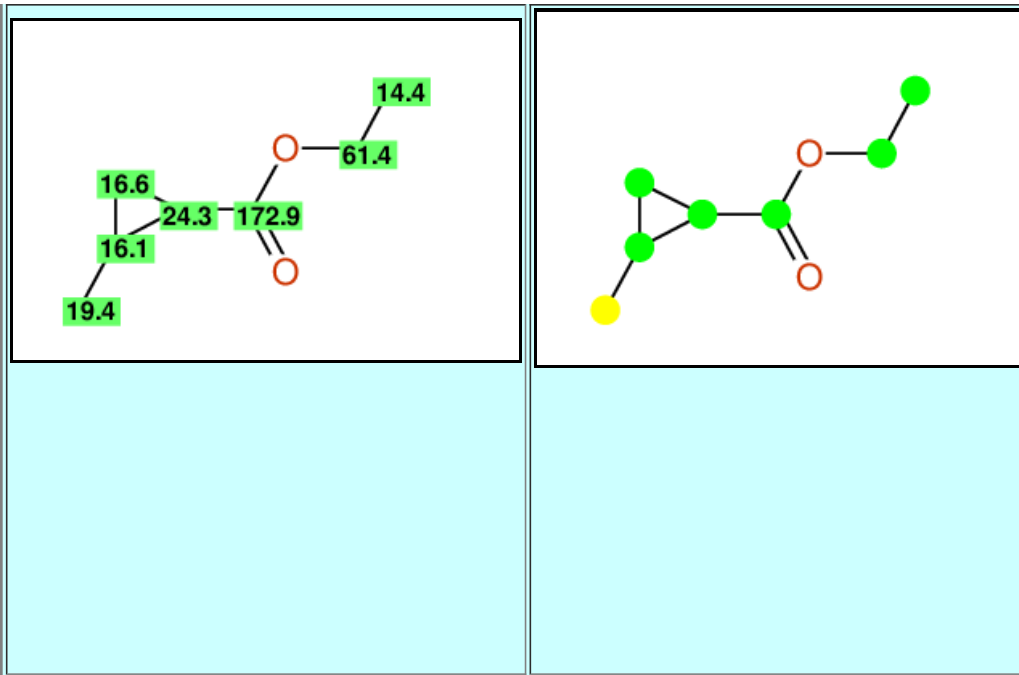
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[Back to Complete Result](#)

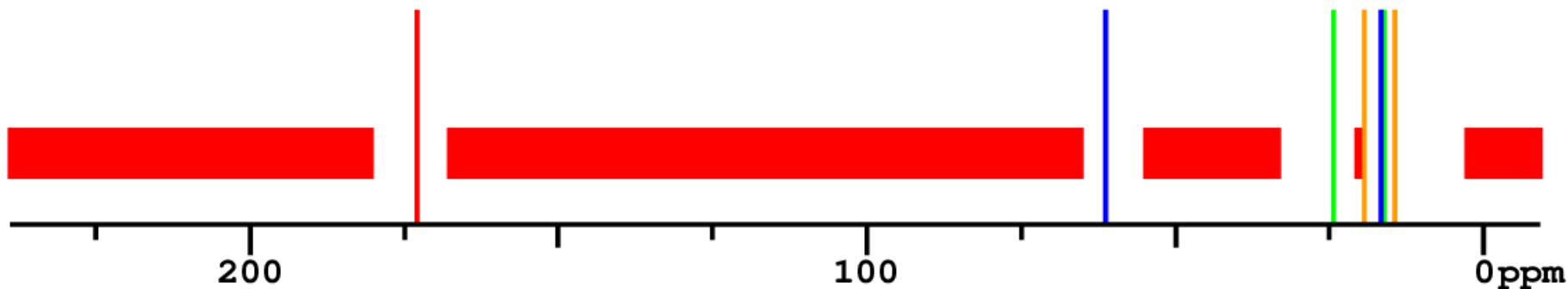
Structure Proposal #3

Structure	Similarity Measure
	<p>Deviation = 2.77 ppm Similarity = 93 %</p> <p>C_7O_2</p> <p>MWT = 116.08</p> <p>Search Web for this structure: ZNXRPIKPYJZPNI</p>
Predicted Chemical Shiftvalues	Matching Map



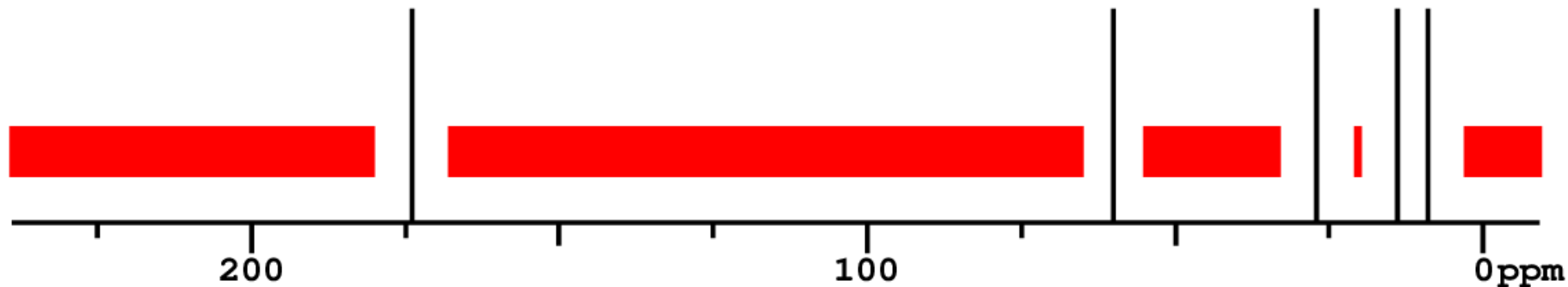
Predicted shift values

Signal multiplicity: S D T Q O E P ?



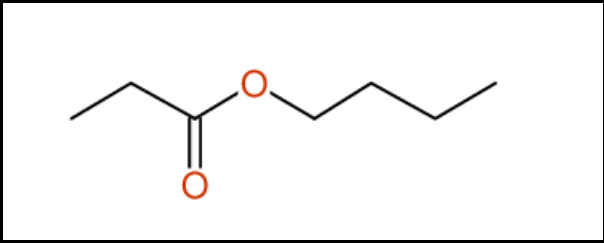
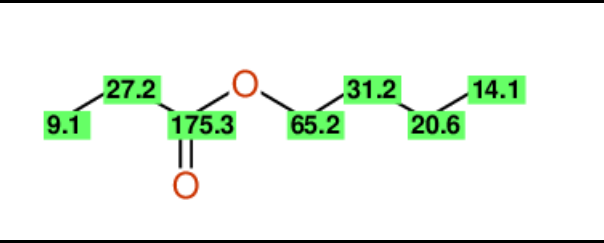
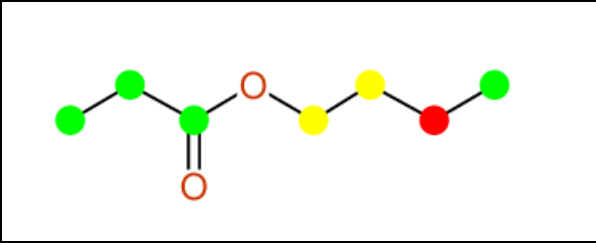
Experimental shift values

No line in reference: 



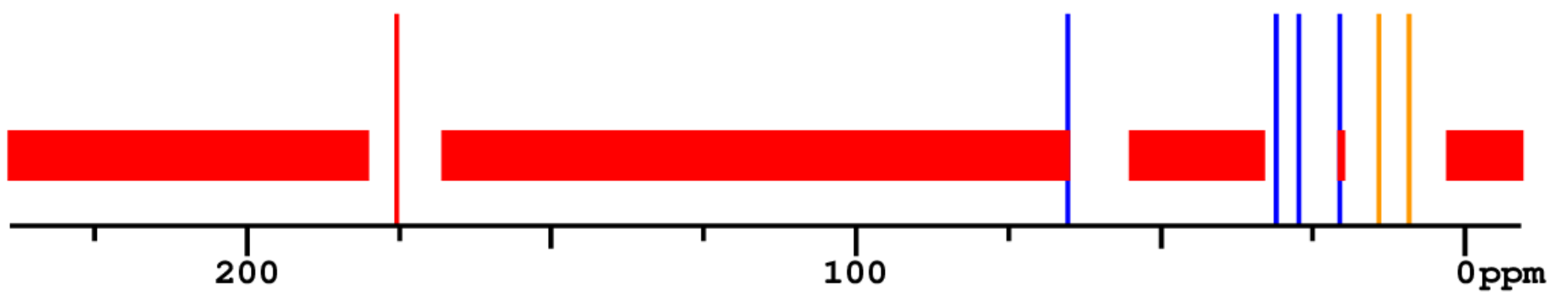
[Back to Complete Result](#)

Structure Proposal #4

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

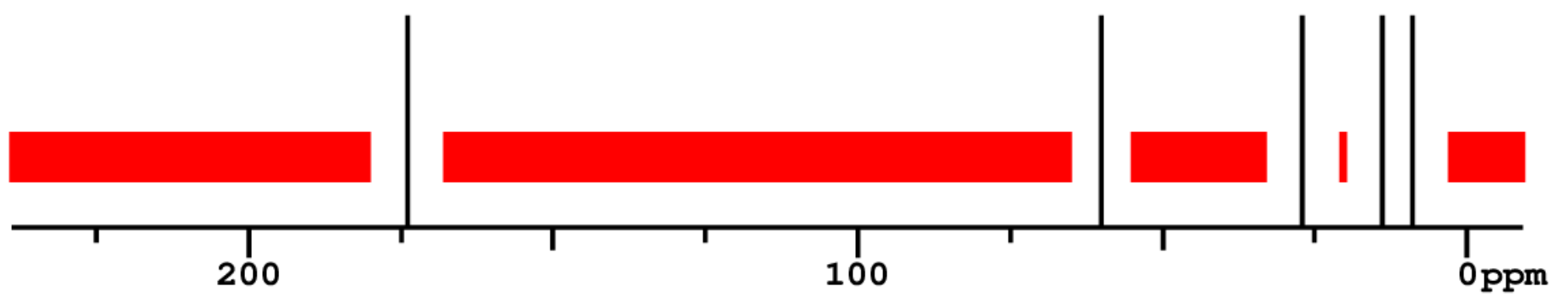
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

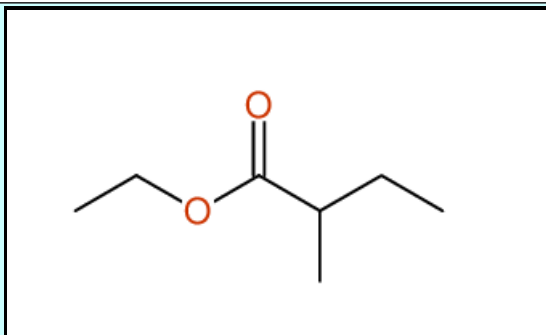
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[Back to Complete Result](#)

Structure Proposal #5

Structure	Similarity Measure



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

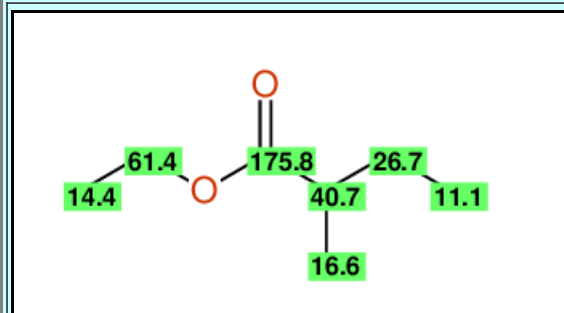
C_7O_2

MWT = 116.08

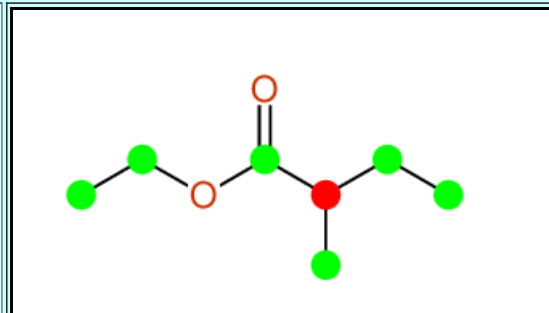
Search Web for this structure:

[JPVJJBICKBKSH](#)

Predicted Chemical Shiftvalues

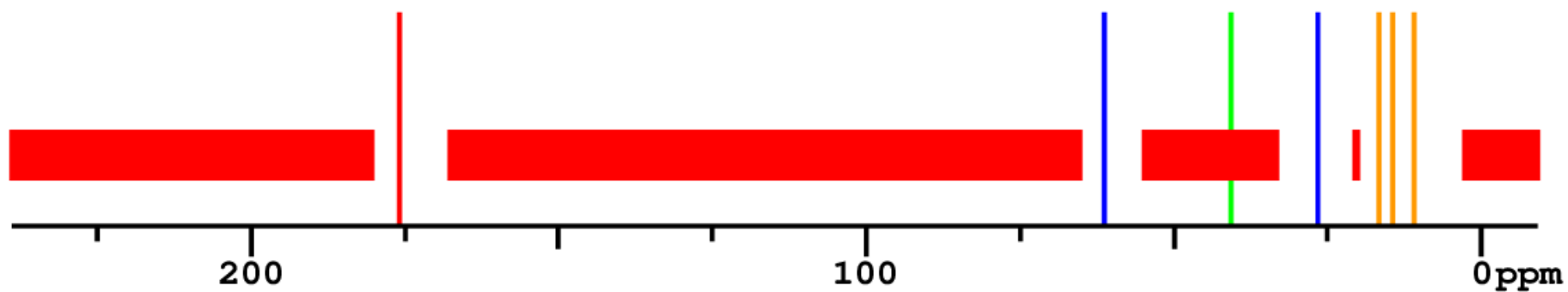


Matching Map



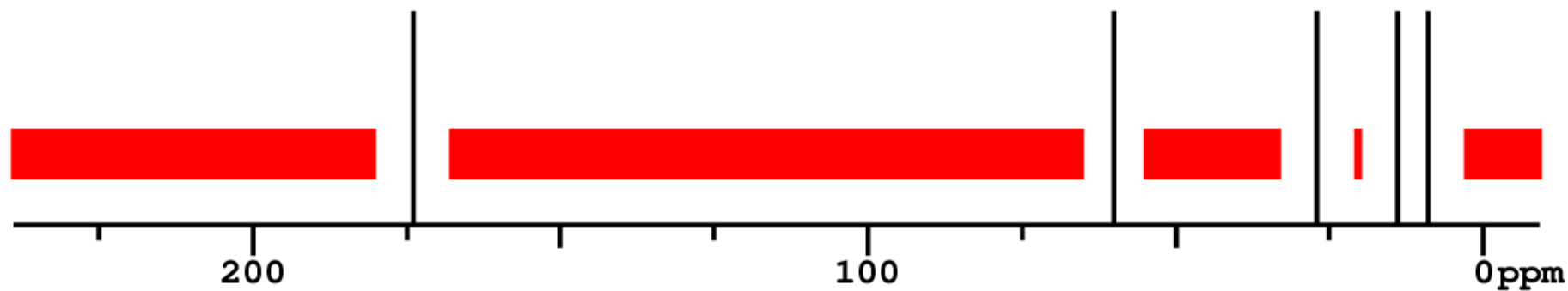
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

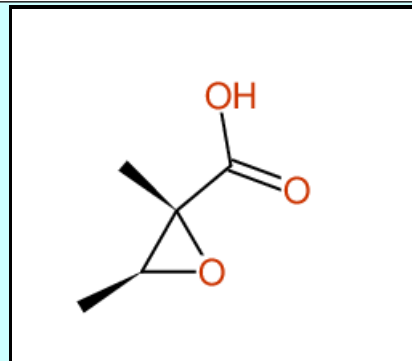
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[Back to Complete Result](#)

Structure Proposal #6

Structure	Similarity Measure



Deviation = 3.54 ppm
Similarity = 70 %
(Different pattern)

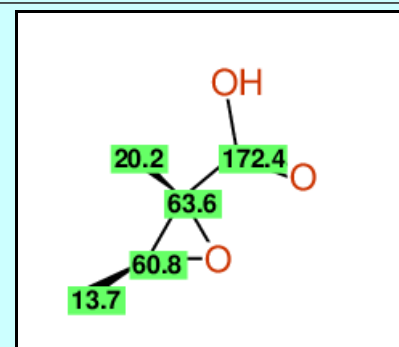


MWT = 108.06

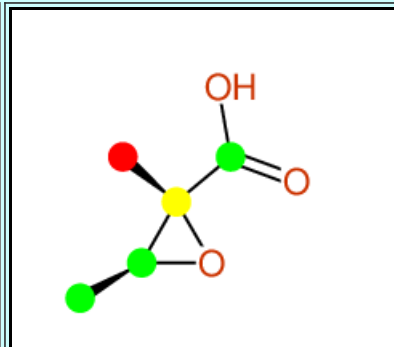
Search Web for this structure:

[RUFMEDUWOSHOHF](#)

Predicted Chemical
Shiftvalues

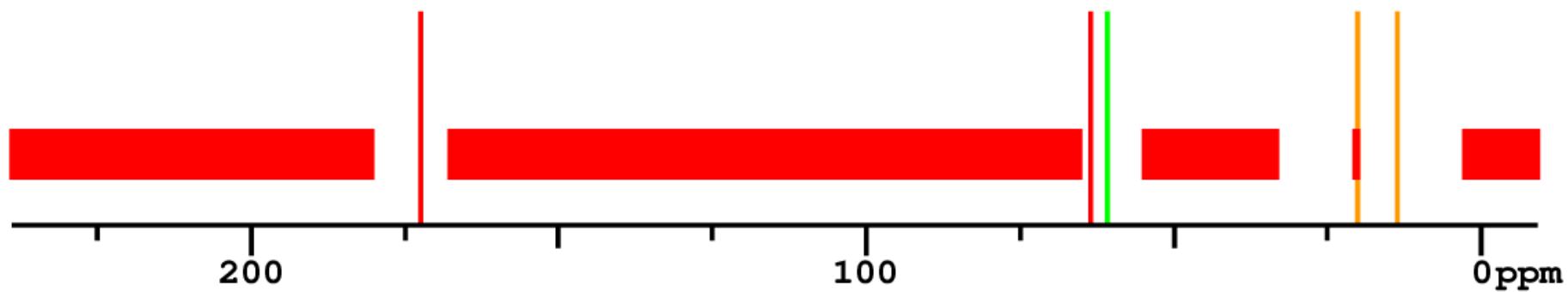


Matching Map



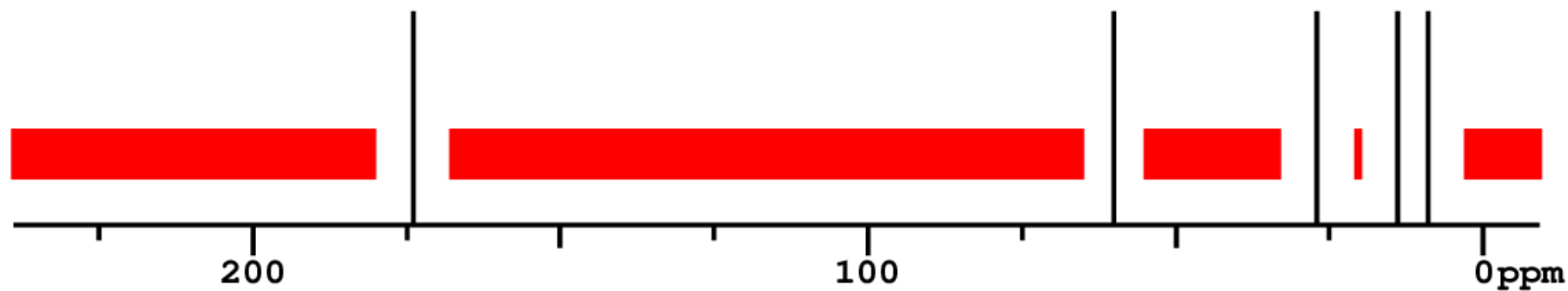
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

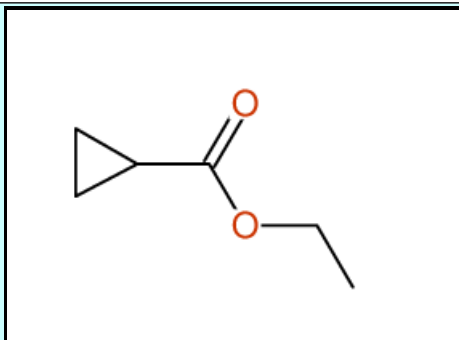
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[Back to Complete Result](#)

Structure Proposal #7

Structure	Similarity Measure



Deviation = 3.54 ppm
Similarity = 100 %

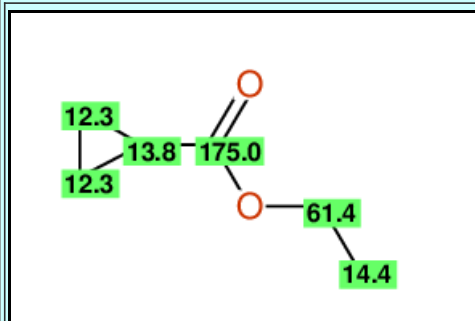
C_6O_2

MWT = 104.07

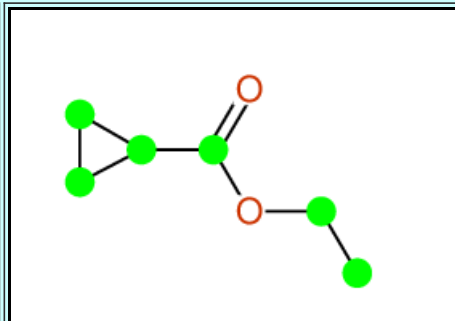
Search Web for this structure:

[OARDGAWFHAUOJC](#)

Predicted Chemical Shiftvalues

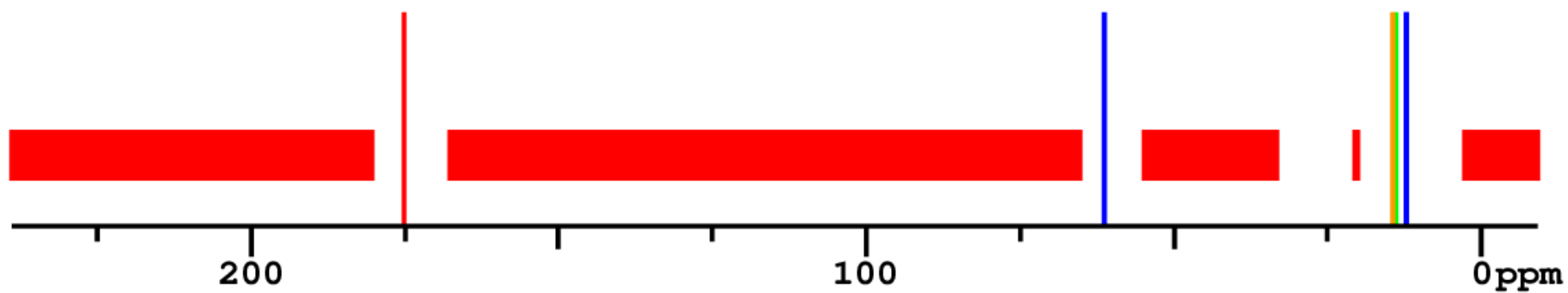


Matching Map



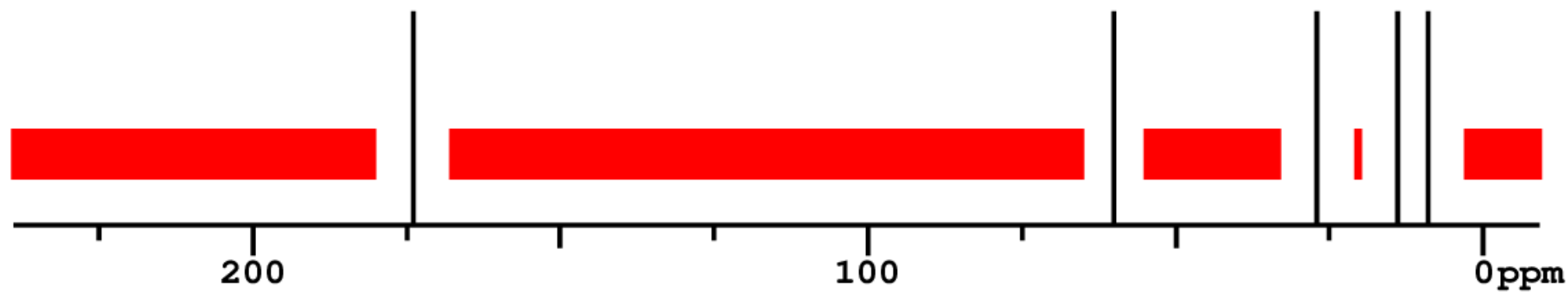
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

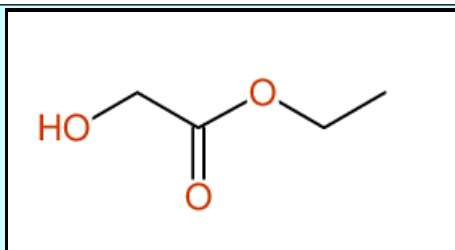
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[Back to Complete Result](#)

Structure Proposal #8

Structure	Similarity Measure



Deviation = 3.72 ppm
Similarity = 100 %

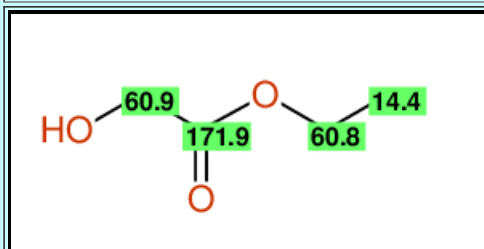
C_4O_3

MWT = 96.04

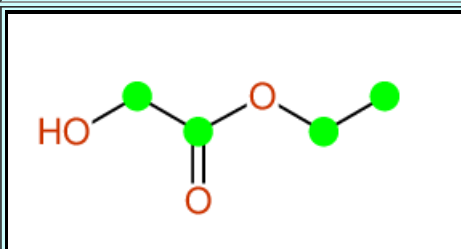
Search Web for this structure:

[USTOPXSKJLOMKG](#)

Predicted Chemical Shiftvalues

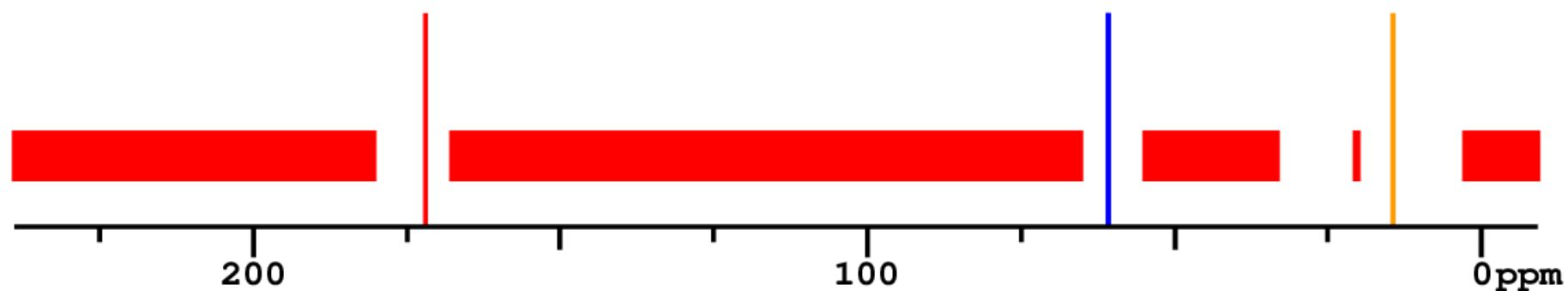


Matching Map



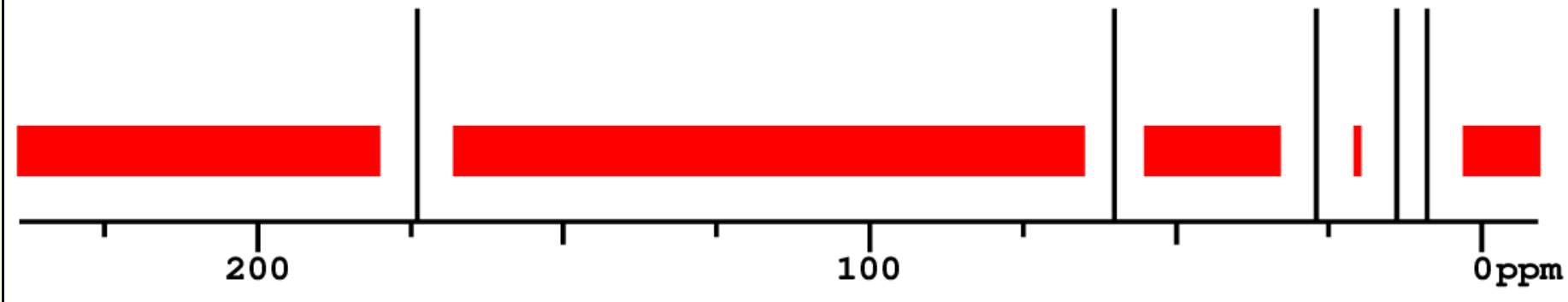
Predicted shift values

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



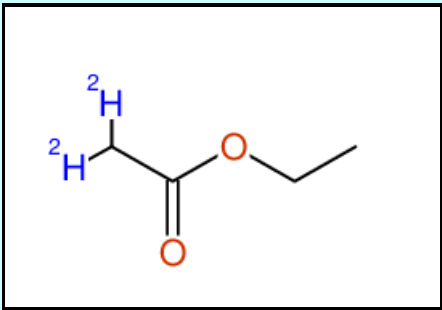
Experimental shift values

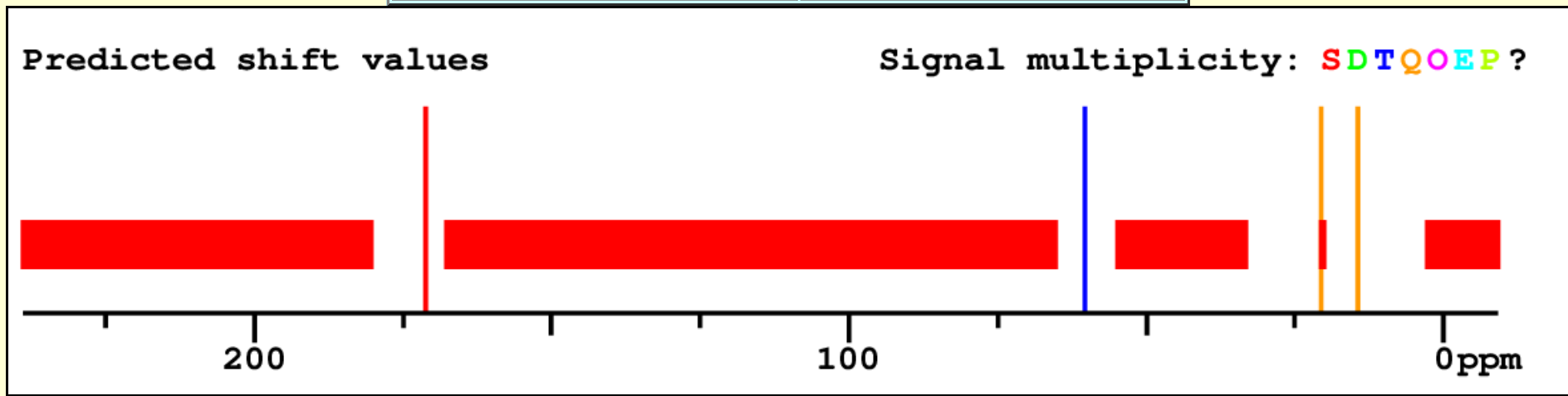
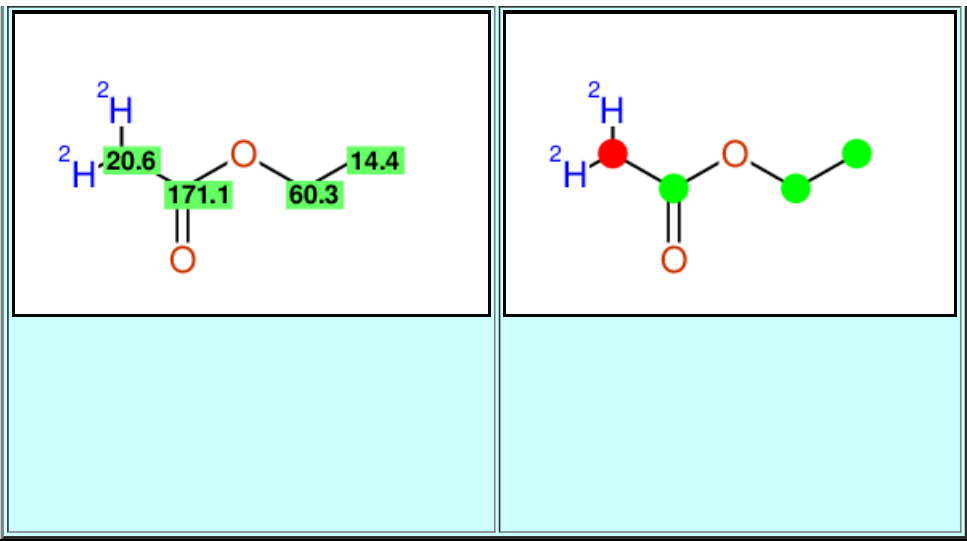
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[Back to Complete Result](#)

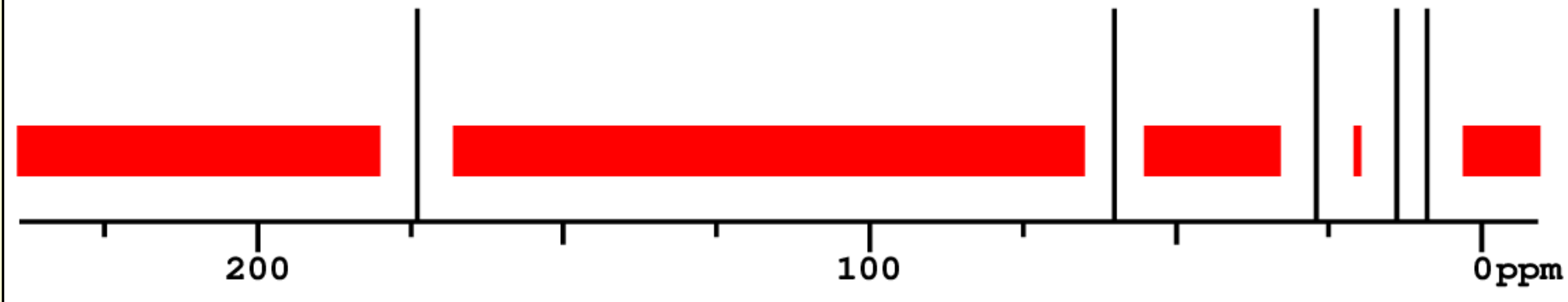
Structure Proposal #9

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



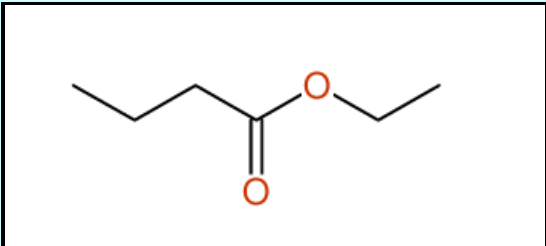
Experimental shift values

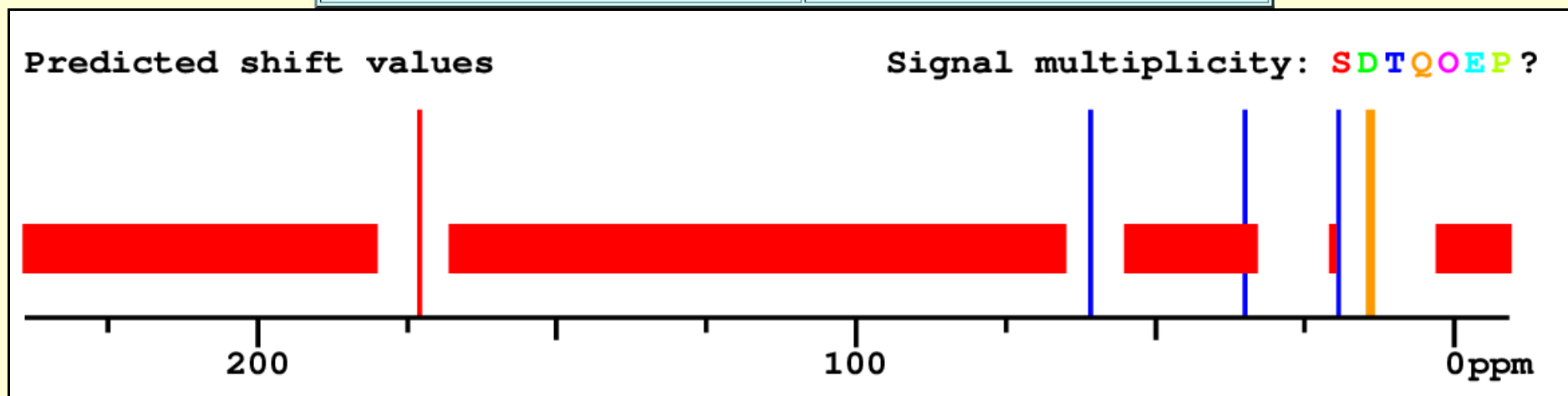
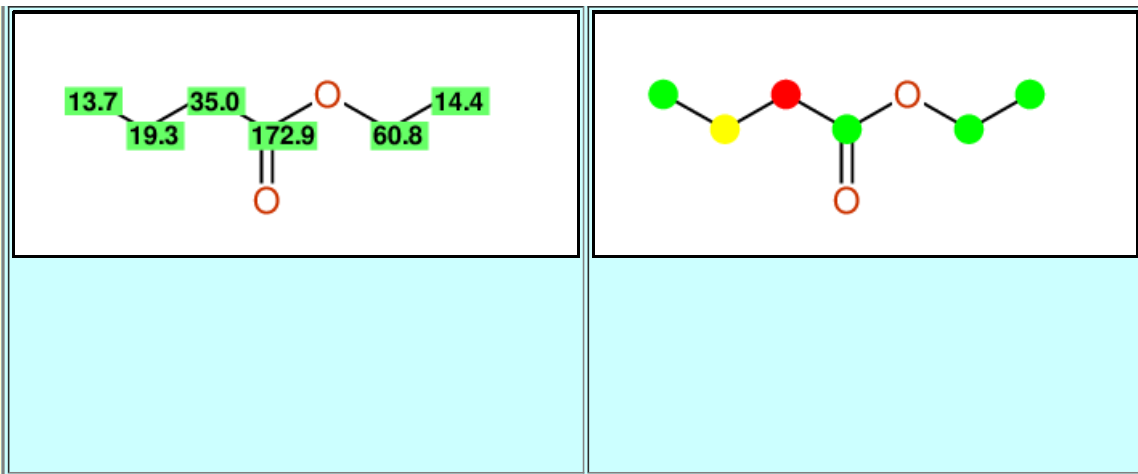
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[Back to Complete Result](#)

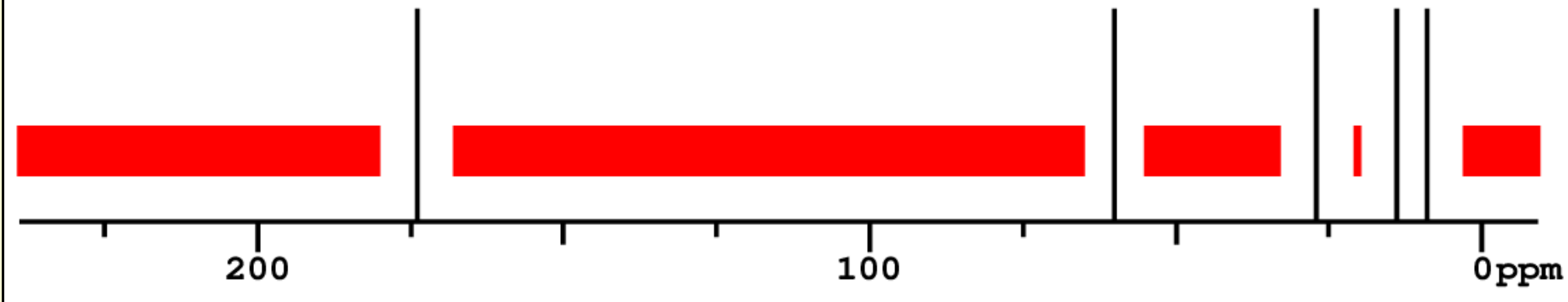
Structure Proposal #10

Structure	Similarity Measure
	<p>Deviation = 4.02 ppm Similarity = 75 % (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 116.07</p> <p>Search Web for this structure: OBNCKNCVKJNDBV Availability</p>
Predicted Chemical Shiftvalues	Matching Map



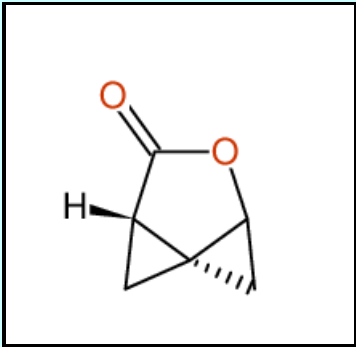
Experimental shift values

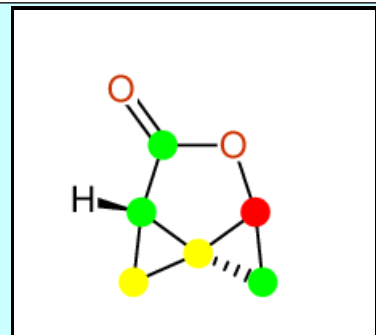
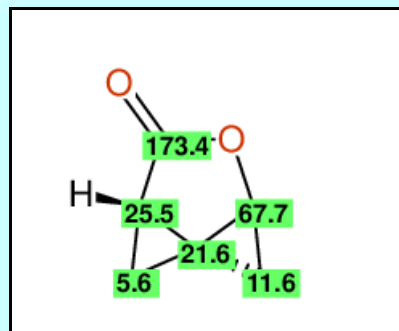
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[Back to Complete Result](#)

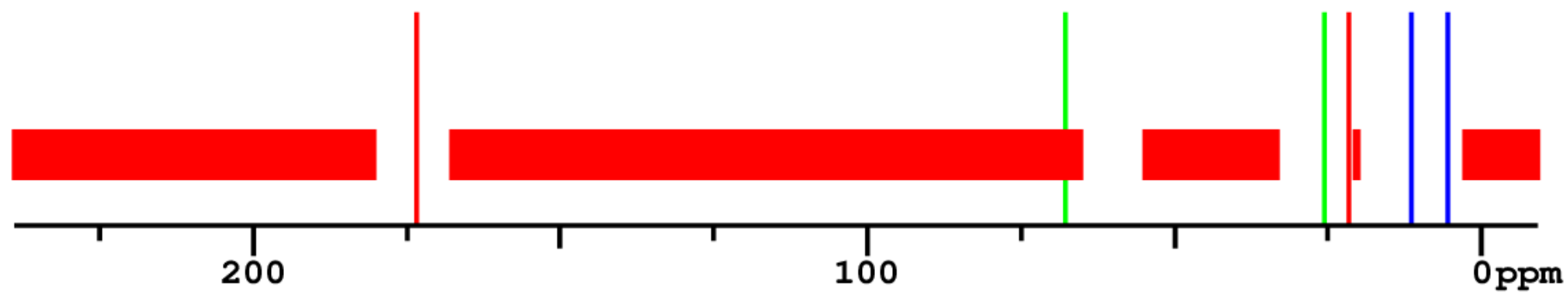
Structure Proposal #11

Structure	Similarity Measure
	<p>Deviation = 4.04 ppm Similarity = 67 % (Different pattern)</p> <p>$C_6H_6O_2$</p> <p>MWT = 110.07</p> <p>Search Web for this structure: WZLNCRVWIKHJER</p>
Predicted Chemical Shiftvalues	Matching Map



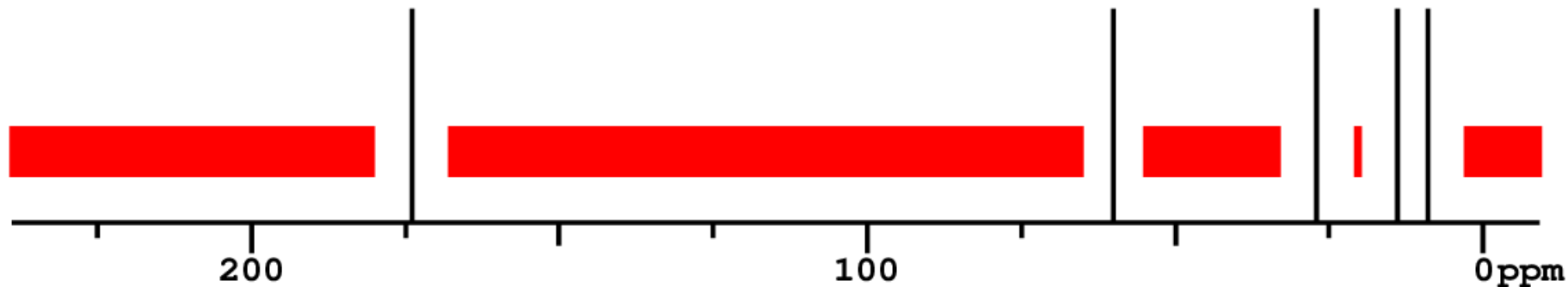
Predicted shift values

Signal multiplicity: S D T Q O E P ?



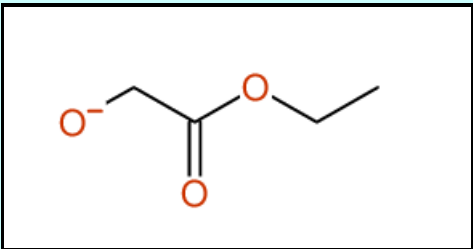
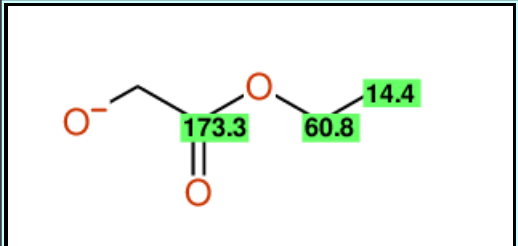
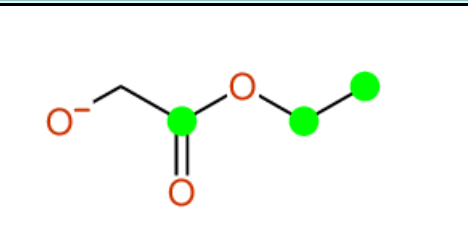
Experimental shift values

No line in reference: 



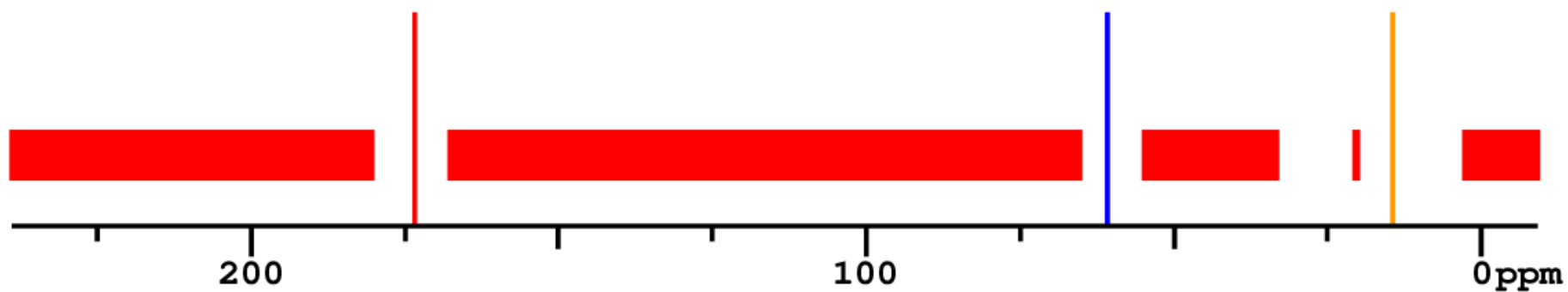
[Back to Complete Result](#)

Structure Proposal #12

Structure	Similarity Measure
	Deviation = 4.11 ppm Similarity = 100 % C ₄ H ₇ O ₃ MWT = 103.04 Search Web for this structure: PDHCCQJYEKLVR
Predicted Chemical Shiftvalues	Matching Map
	

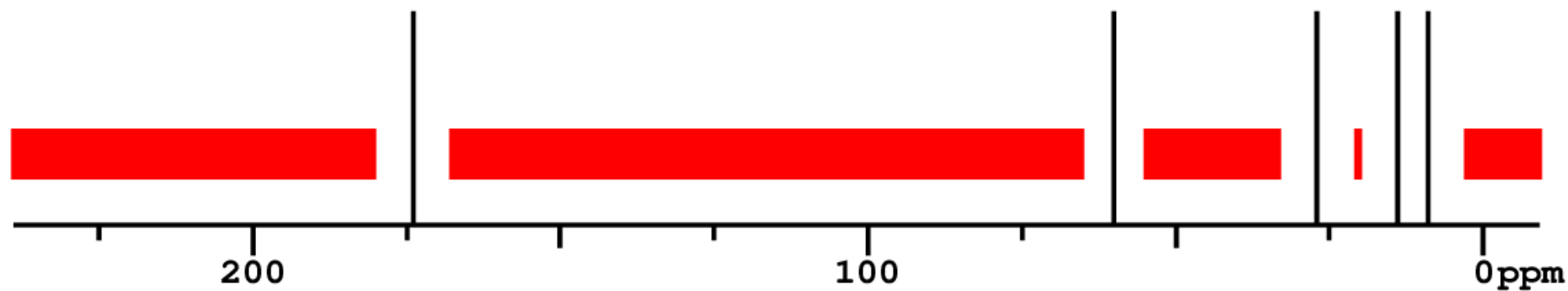
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

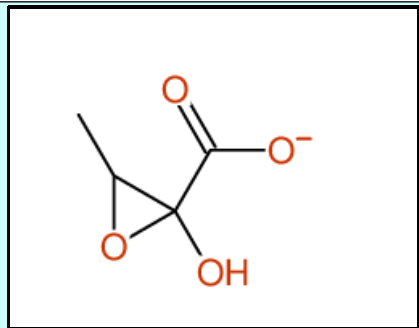
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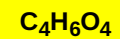
[Back to Complete Result](#)

Structure Proposal #13

Structure	Similarity Measure



Deviation = 4.23 ppm
Similarity = 100 %

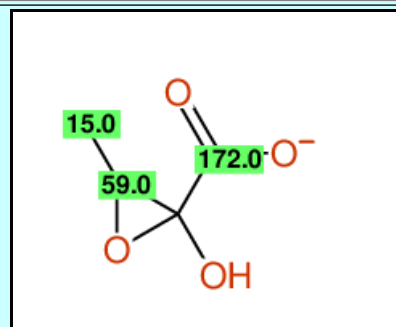


MWT = 118.04

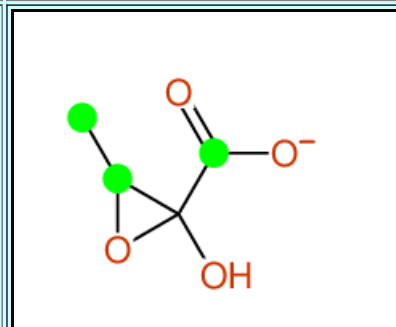
Search Web for this structure:

[KYFIXARGJXDEJJ](#)

Predicted Chemical
Shiftvalues

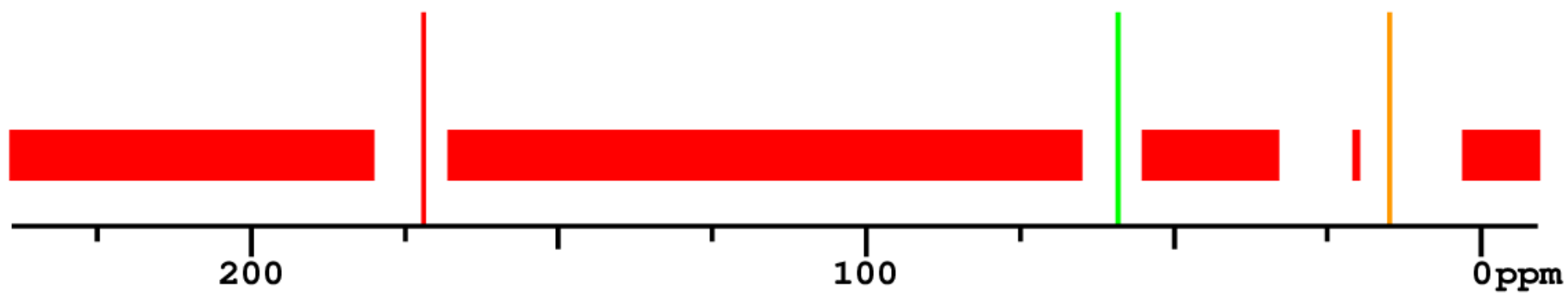


Matching Map



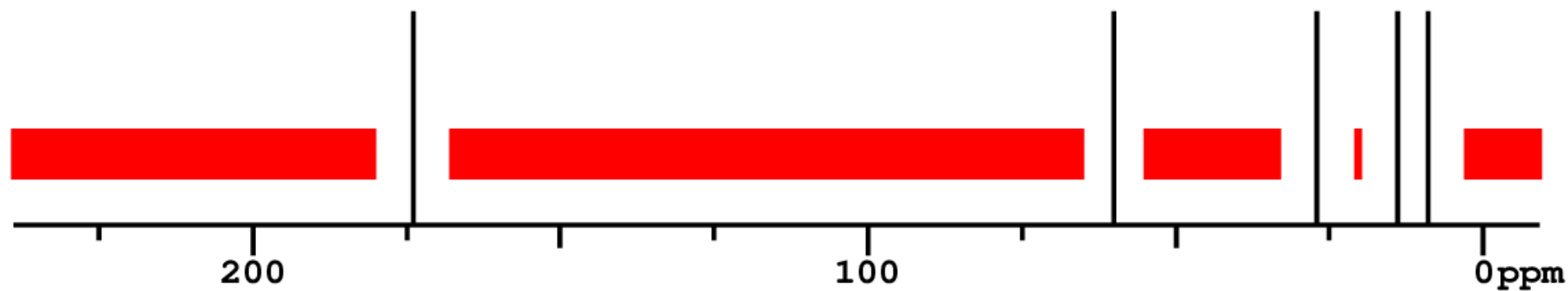
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

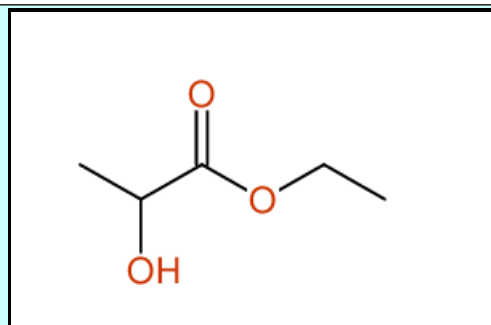
No line in reference: [red bar]



[Back to Complete Result](#)

Structure Proposal #14

Structure	Similarity Measure



Deviation = 4.33 ppm
 Similarity = 70 %
 (Different pattern)

C_5O_3

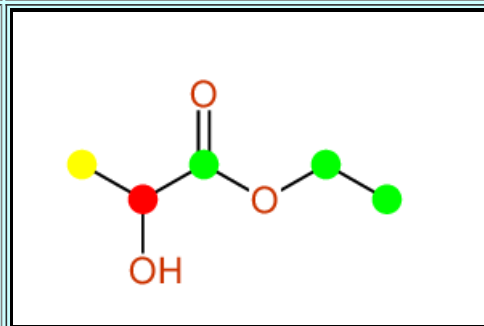
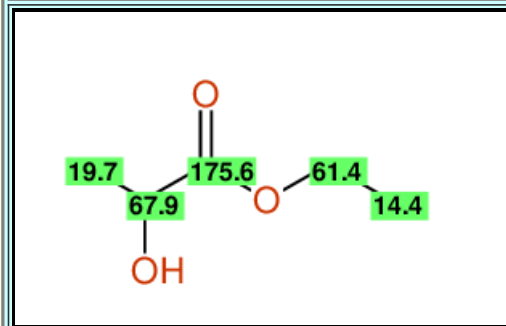
MWT = 108.06

Search Web for this structure:

[FPXAEZNSBIYEJ](#)

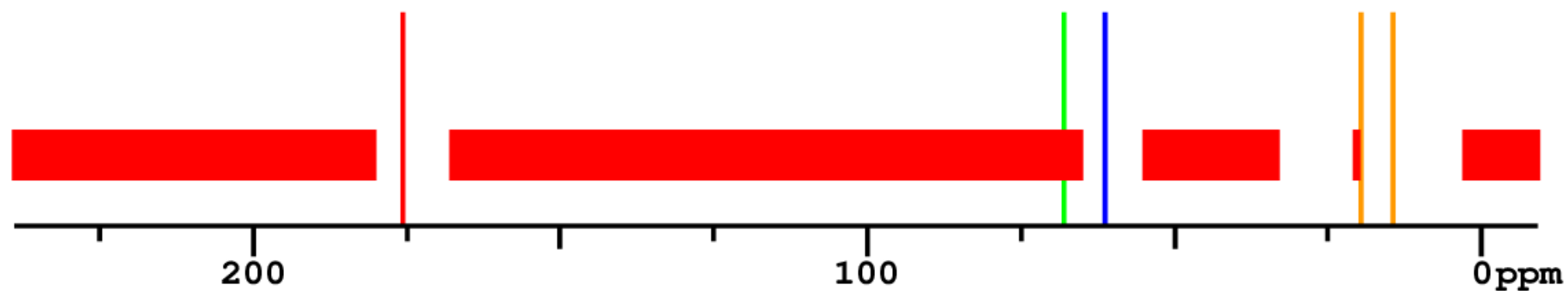
Predicted Chemical Shiftvalues

Matching Map



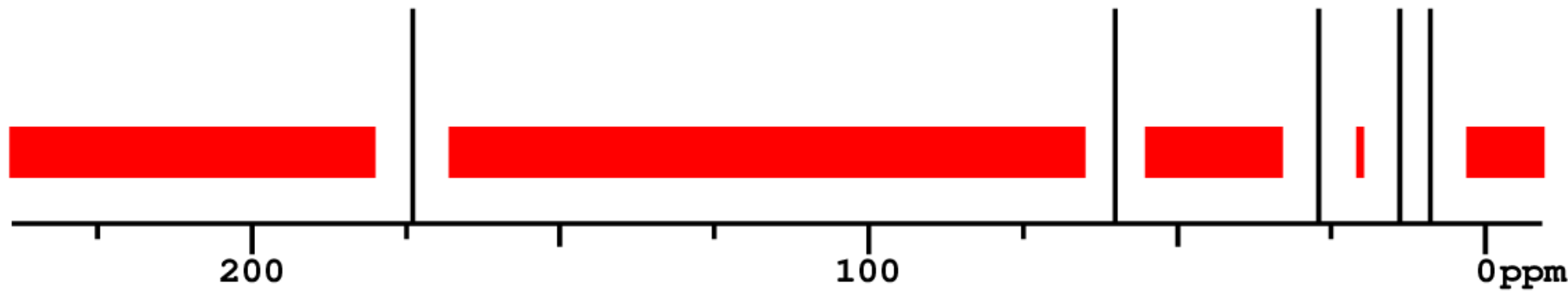
Predicted shift values

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



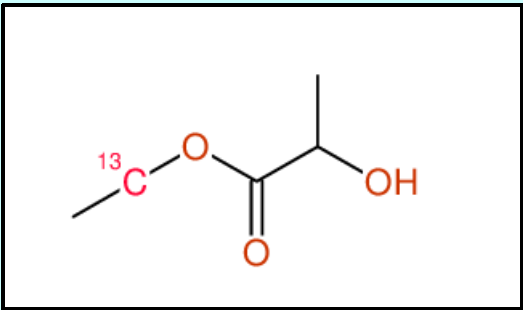
Experimental shift values

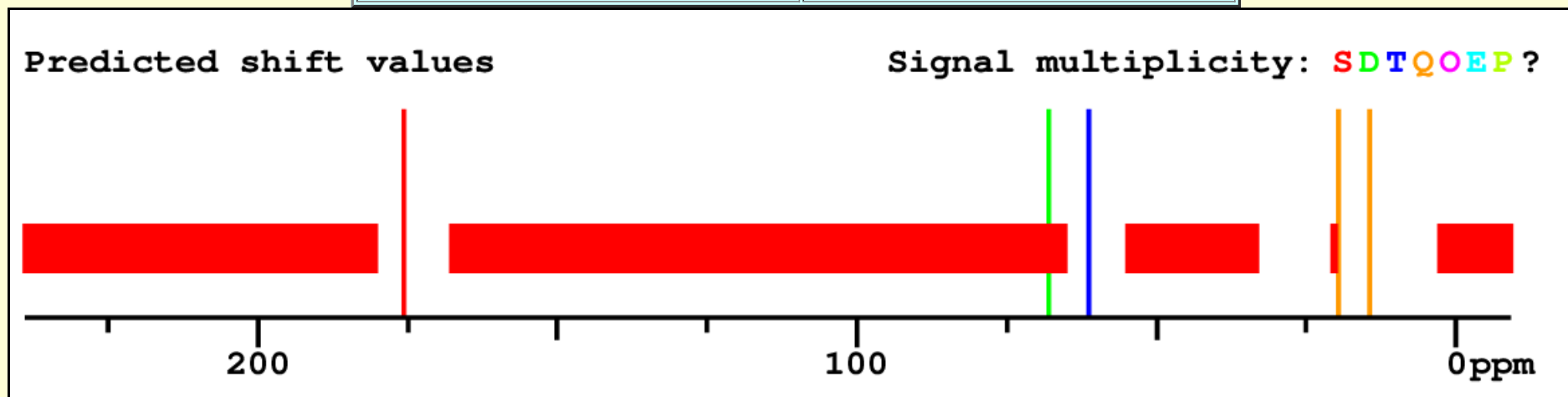
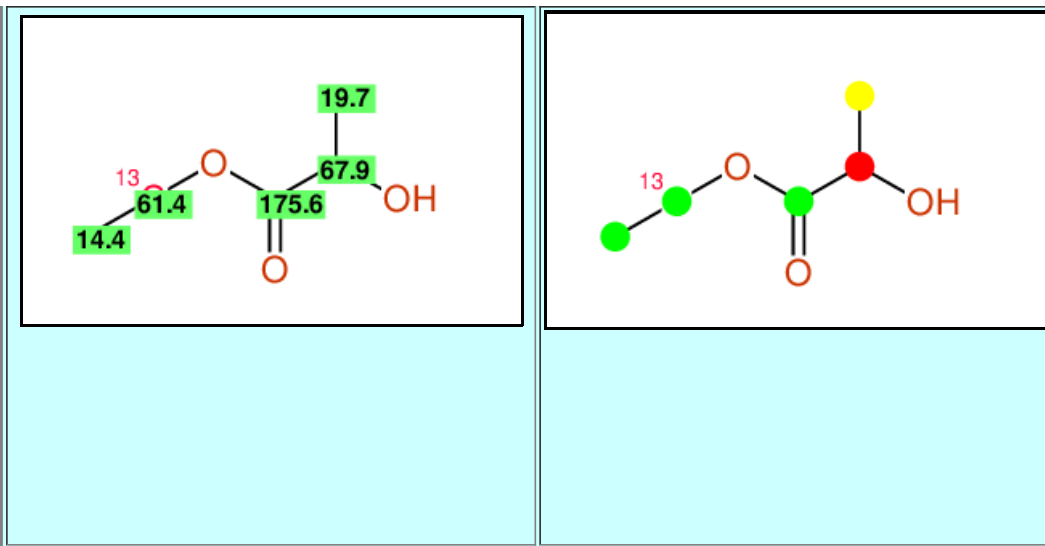
No line in reference: 



[Back to Complete Result](#)

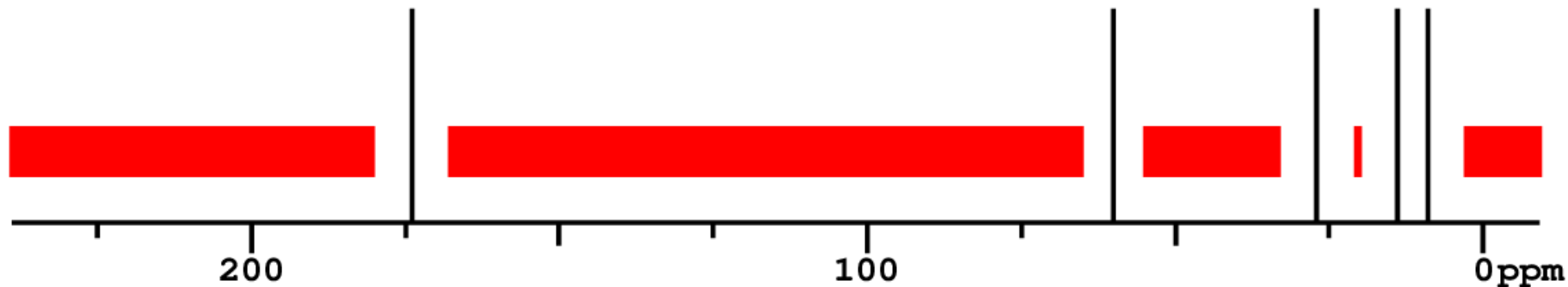
Structure Proposal #15

Structure	Similarity Measure
 <p>The chemical structure shows methyl 2-hydroxypropanoate. The methyl carbon is labeled with a red '13C'. The structure includes a methyl group, an ester oxygen, a carbonyl group, a chiral center with a hydroxyl group, and another methyl group.</p>	<p>Deviation = 4.33 ppm Similarity = 70 % (Different pattern)</p> <p>$C_5H_{10}O_3$</p> <p>MWT = 119.06</p> <p>Search Web for this structure: LZCLXQDLBQLTDK</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



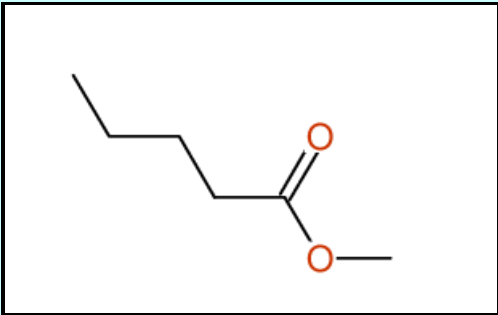
Experimental shift values

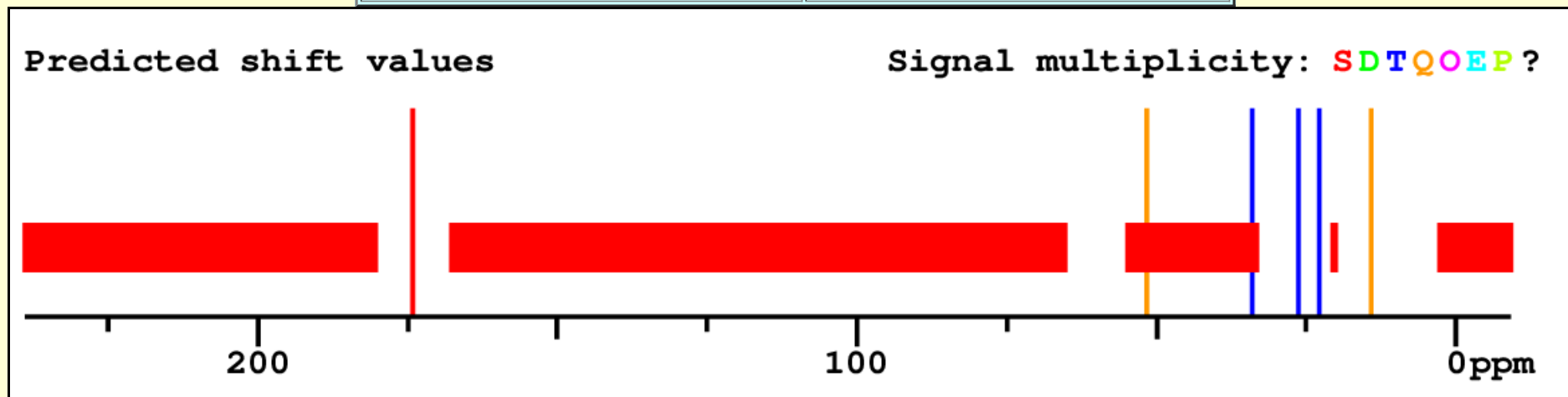
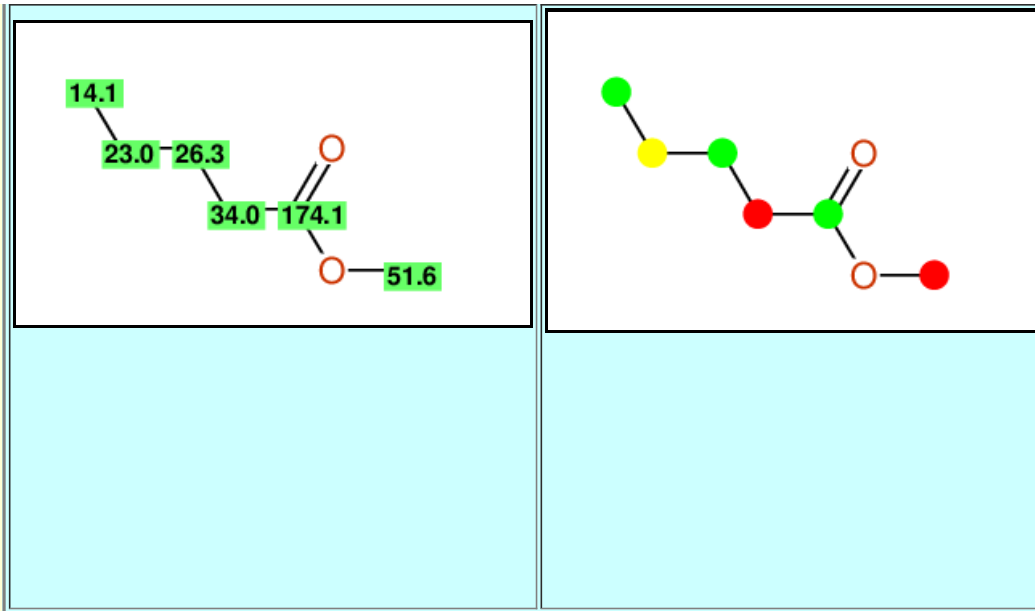
No line in reference: 



[Back to Complete Result](#)

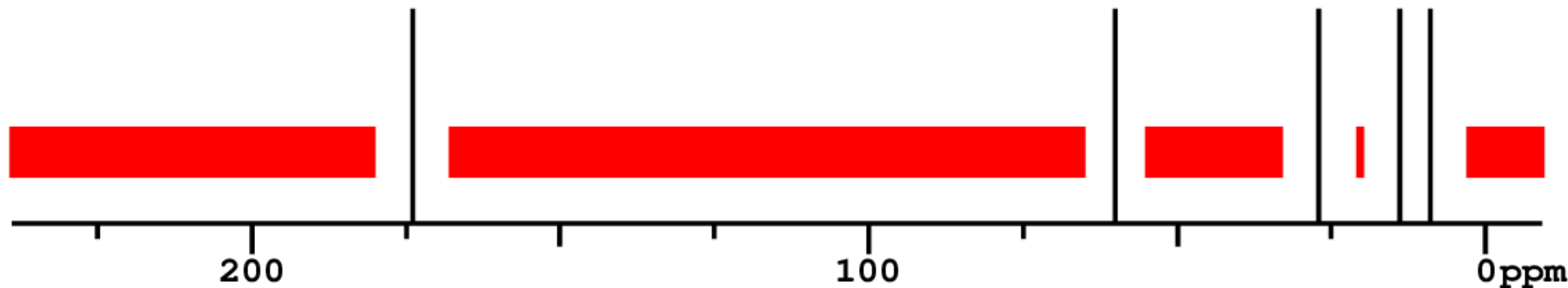
Structure Proposal #16

Structure	Similarity Measure
	<p>Deviation = 4.57 ppm Similarity = 58 % (Different pattern)</p> <p>C_6O_2</p> <p>MWT = 104.07</p> <p>Search Web for this structure: MHBOACTUGJRRKE</p>
Predicted Chemical Shiftvalues	Matching Map



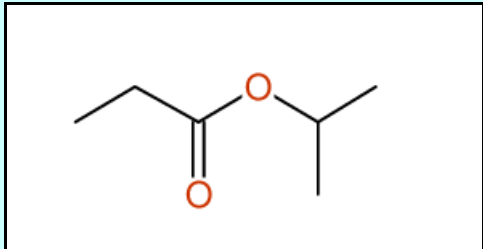
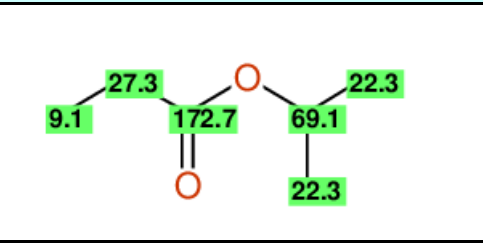
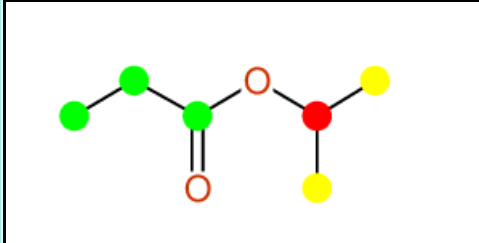
Experimental shift values

No line in reference: 



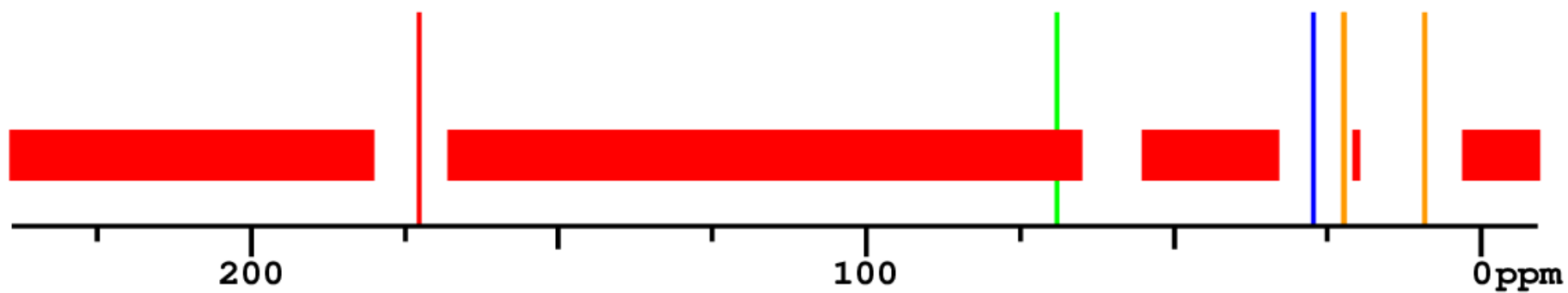
[Back to Complete Result](#)

Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 4.65 ppm Similarity = 67 % (Different pattern)</p> <p>C_6O_2</p> <p>MWT = 104.07</p> <p>Search Web for this structure: IMNXURKAQGHYAH</p>
Predicted Chemical Shiftvalues	Matching Map
	

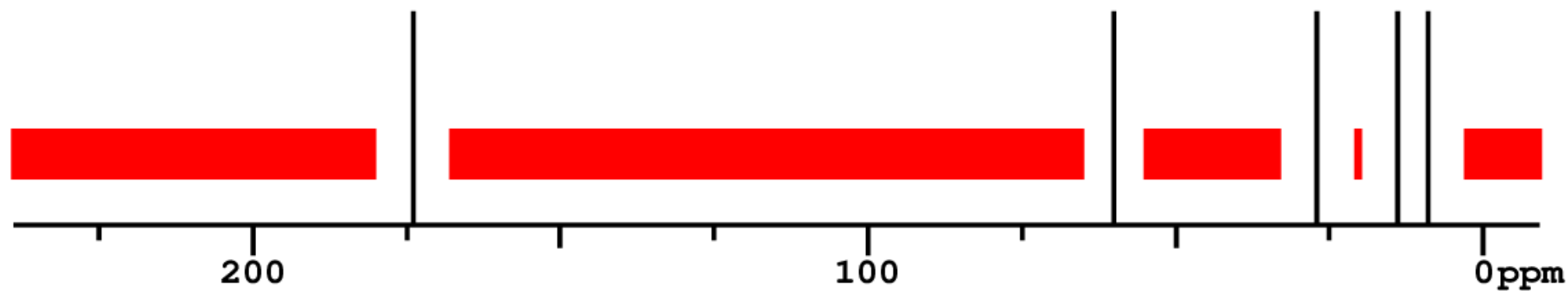
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

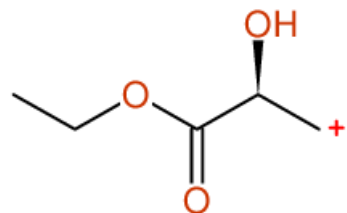
No line in reference: [red bar]



[Back to Complete Result](#)

Structure Proposal #18

Structure	Similarity Measure



Deviation = 4.70 ppm
Similarity = 100 %

$C_5H_9O_3$

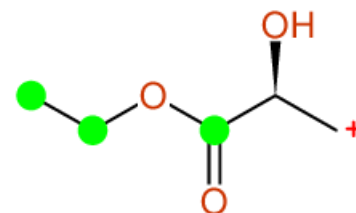
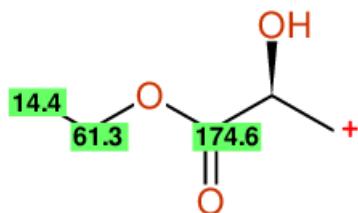
MWT = 117.06

Search Web for this structure:

[SFMRLHJNHWEFDX](#)

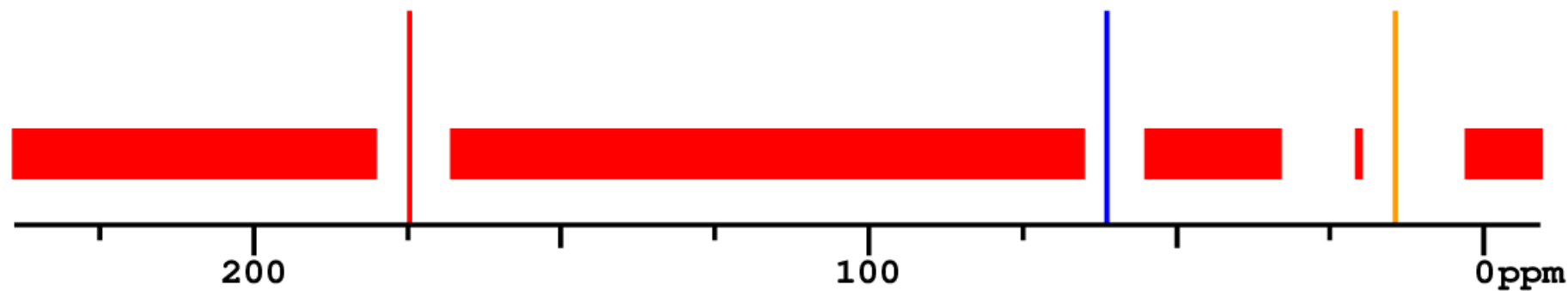
Predicted Chemical Shiftvalues

Matching Map



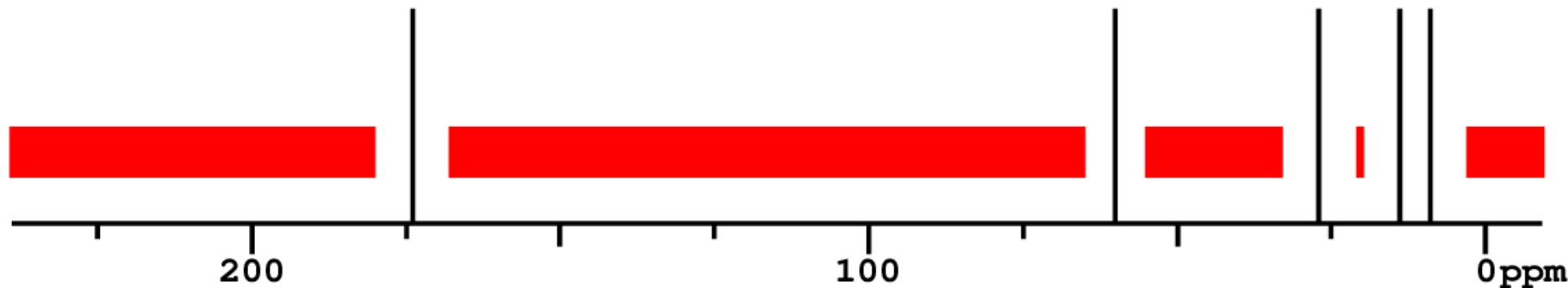
Predicted shift values

Signal multiplicity: S D T Q O E P ?



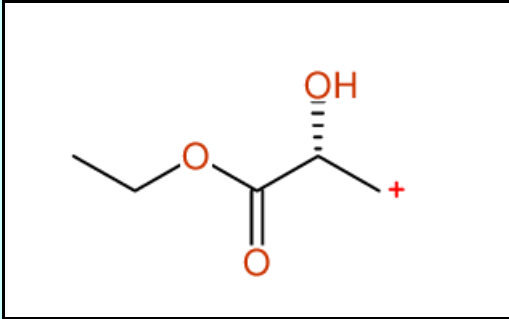
Experimental shift values

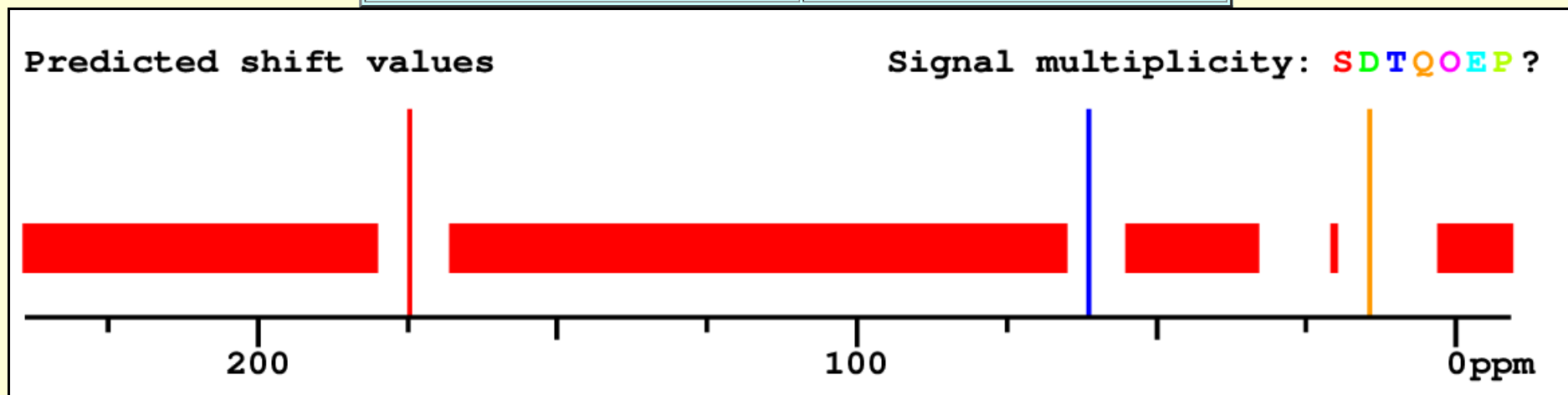
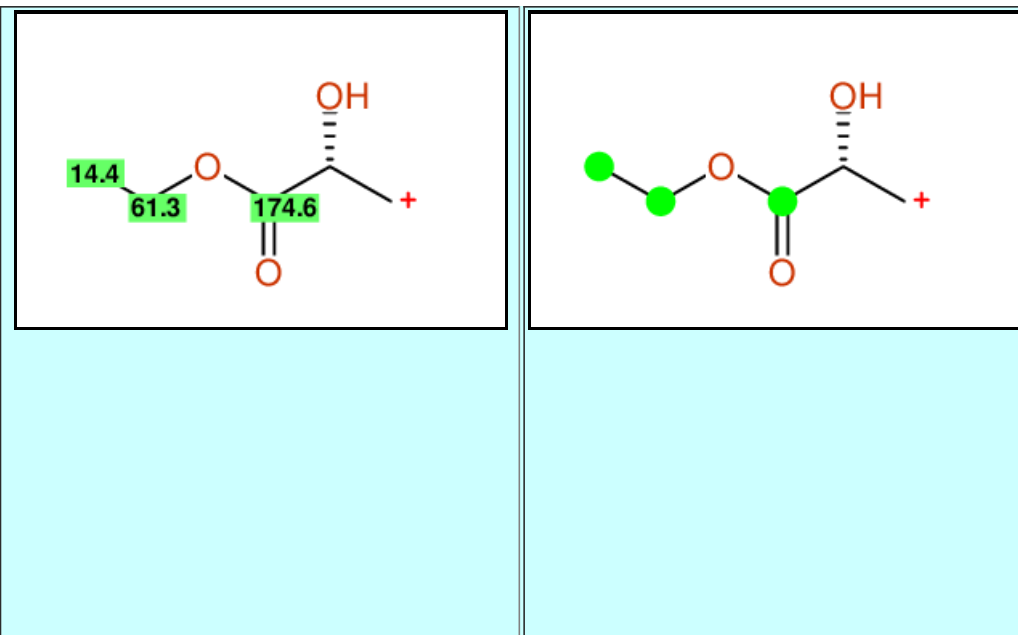
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[Back to Complete Result](#)

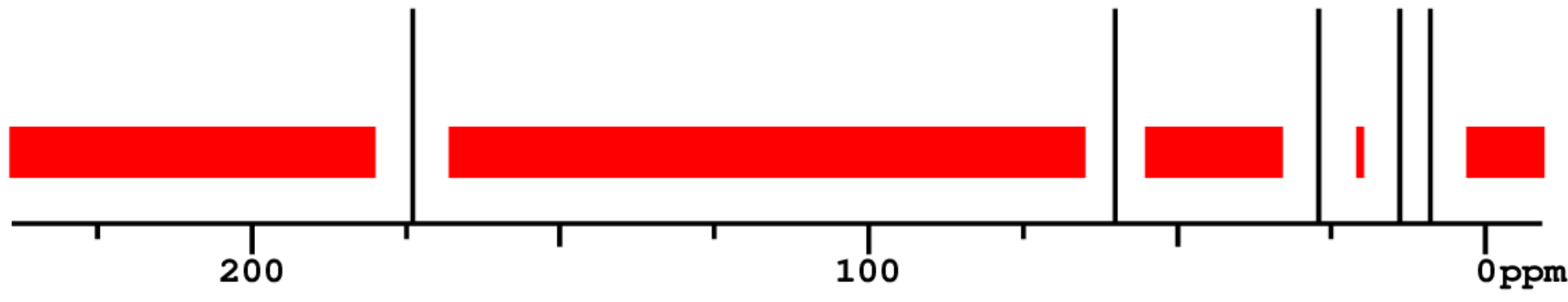
Structure Proposal #19

Structure	Similarity Measure
	Deviation = 4.70 ppm Similarity = 100 % C ₅ H ₉ O ₃ MWT = 117.06 Search Web for this structure: SFMRLHJNHWEFDX
Predicted Chemical Shiftvalues	Matching Map



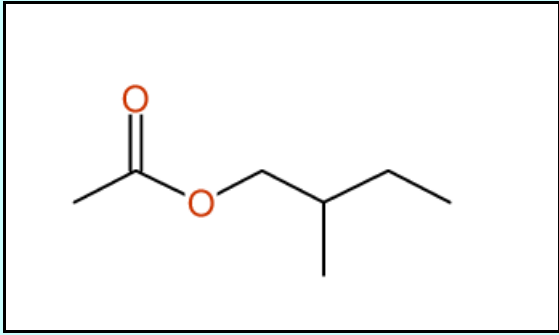
Experimental shift values

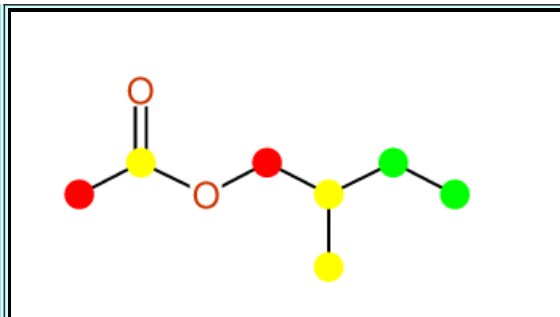
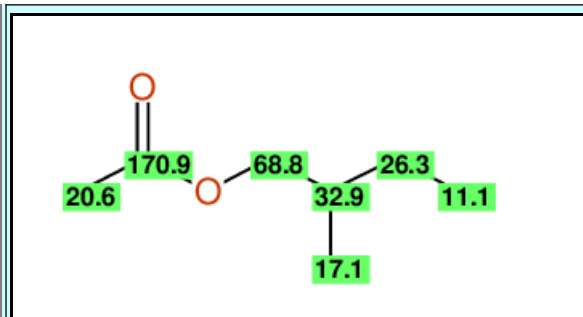
No line in reference: 



[Back to Complete Result](#)

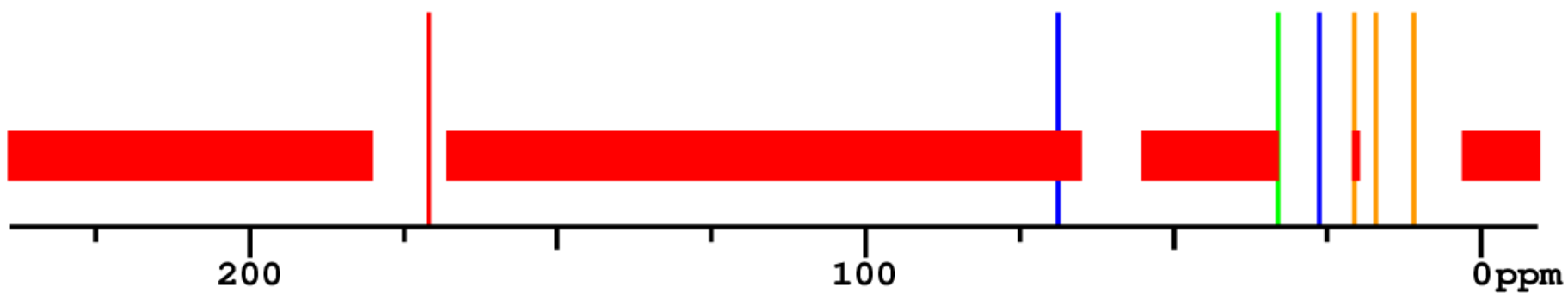
Structure Proposal #20

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



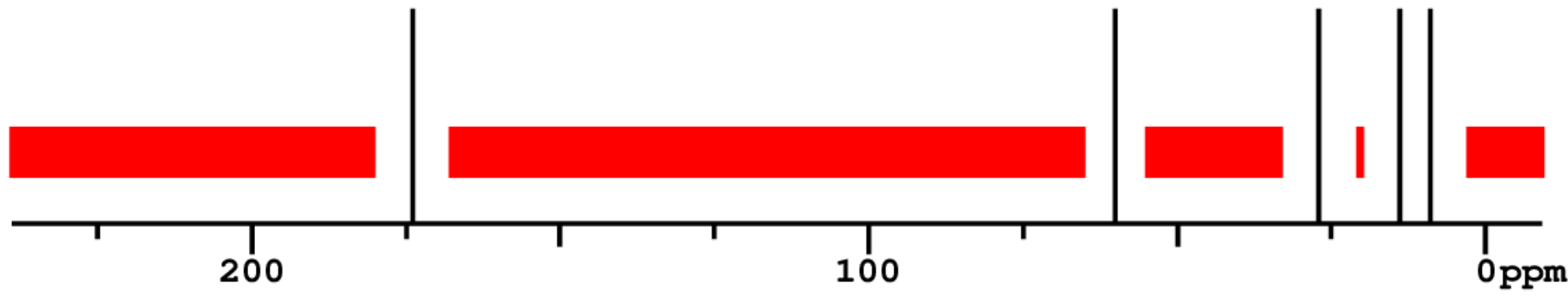
Predicted shift values

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



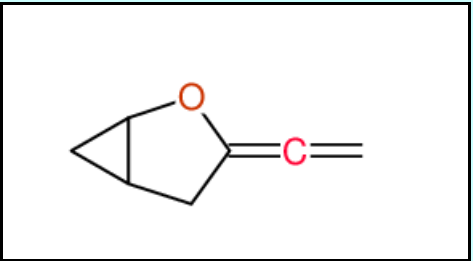
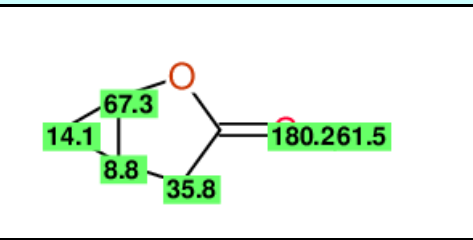
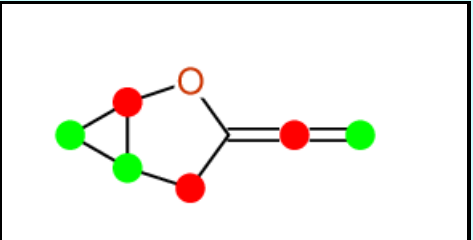
Experimental shift values

No line in reference: 



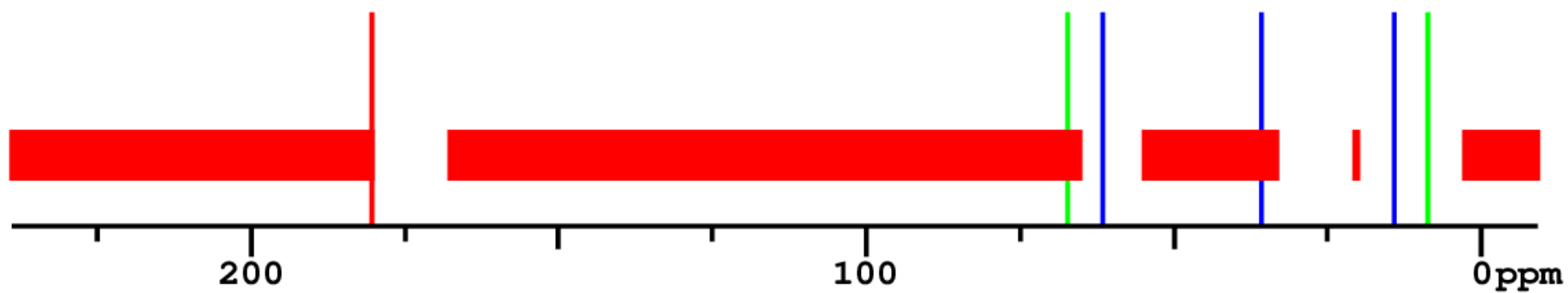
[Back to Complete Result](#)

Structure Proposal #21

Structure	Similarity Measure
	<p>Deviation = 5.23 ppm Similarity = 50 % (Different pattern)</p> <p>C_7H_8O</p> <p>MWT = 108.08</p> <p>Search Web for this structure: HPLLJBRTSULDDV</p>
Predicted Chemical Shiftvalues	Matching Map
	

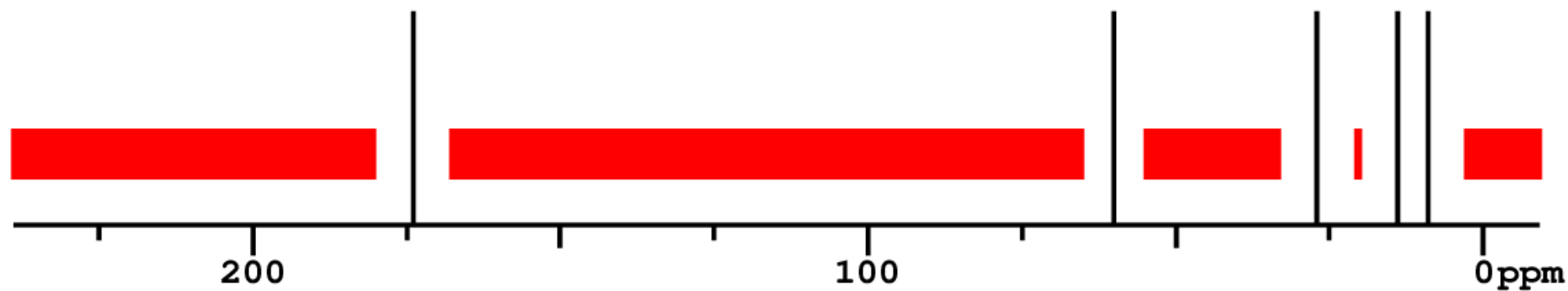
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

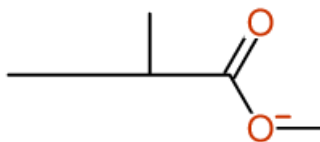
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[Back to Complete Result](#)

Structure Proposal #22

Structure	Similarity Measure



Deviation = 5.23 ppm
Similarity = 67 %
(Different pattern)



MWT = 116.07

Search Web for this structure:

[DREXZGTZFACURE](#)

Predicted Chemical Shiftvalues

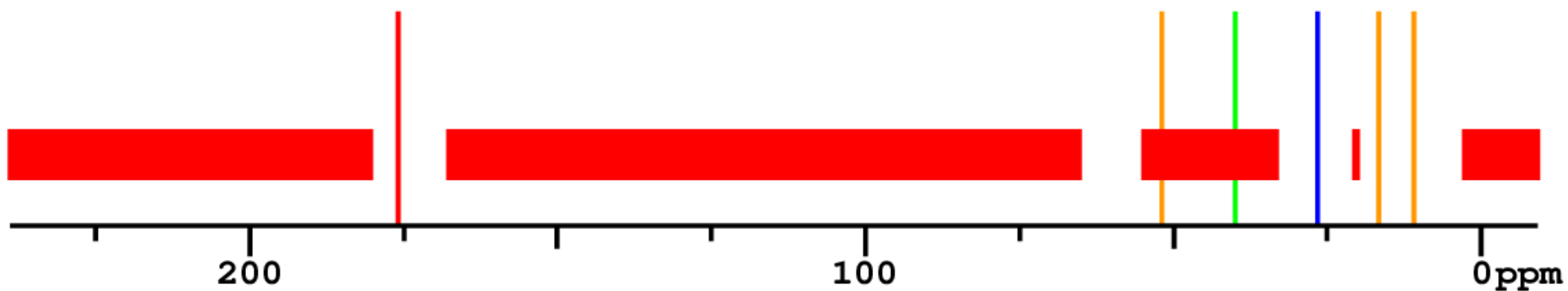


Matching Map



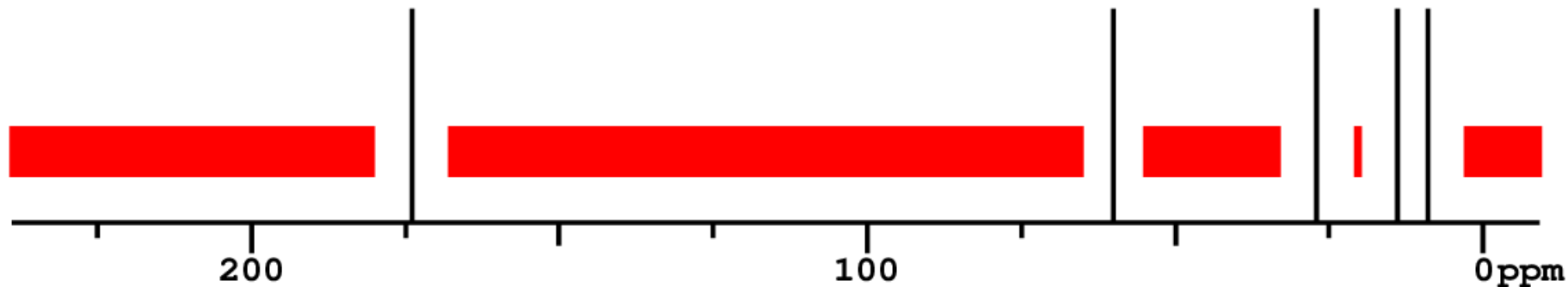
Predicted shift values

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



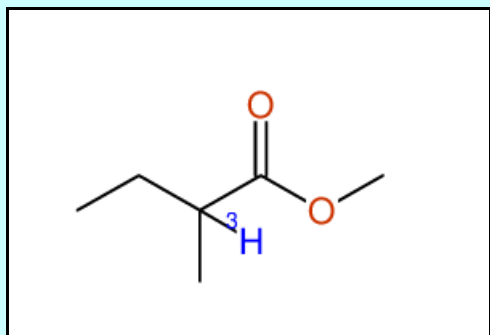
Experimental shift values

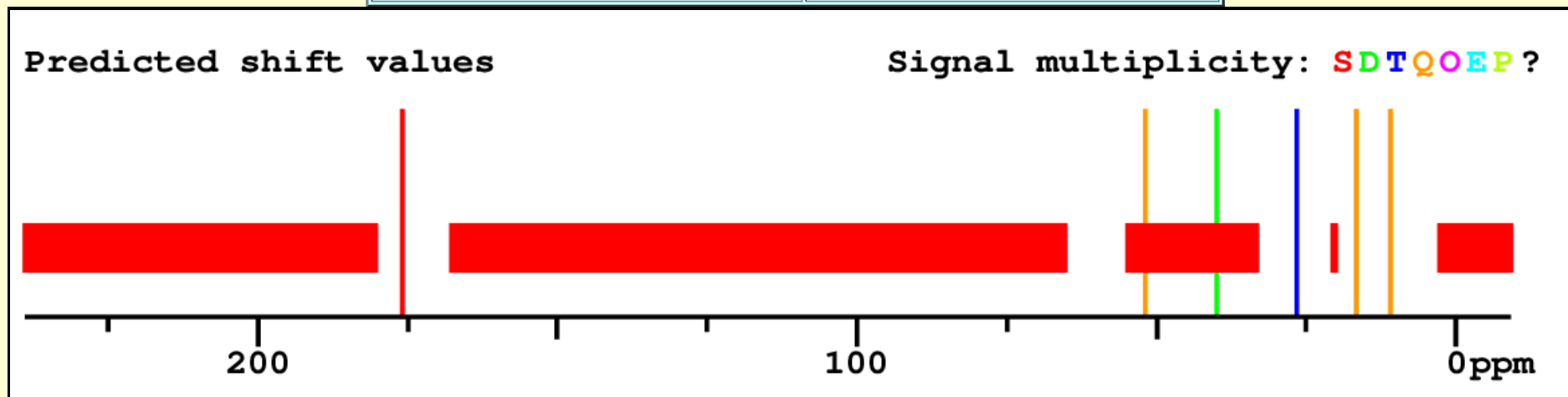
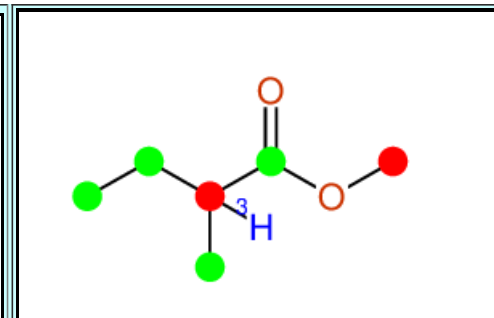
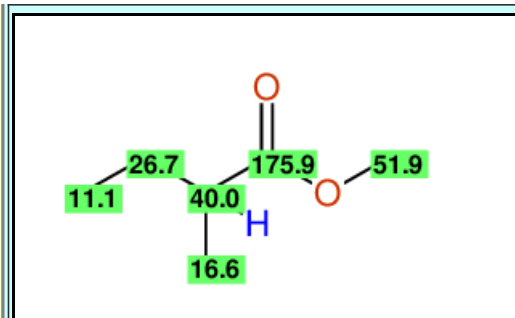
No line in reference: 



[Back to Complete Result](#)

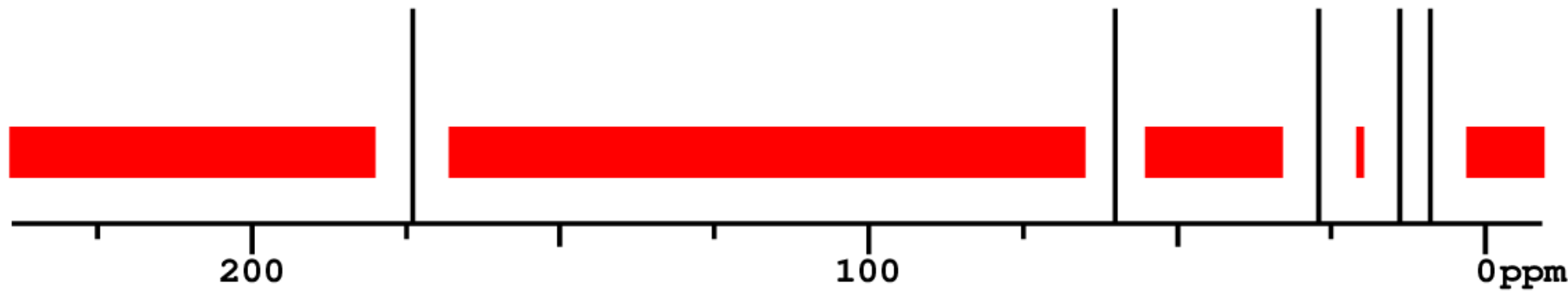
Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm Similarity = 67 % (Different pattern)</p> <p>$C_6H_{12}O_2$</p> <p>MWT = 118.07</p> <p>Search Web for this structure: OCWLYWIFENDCWRZ</p> <p>Availability</p>
Predicted Chemical Shiftvalues	Matching Map



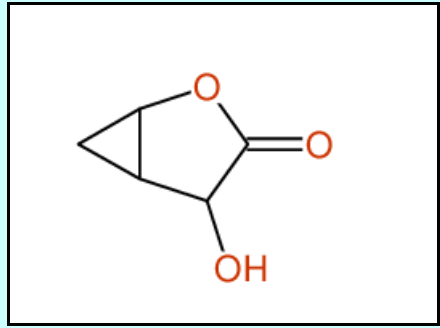
Experimental shift values

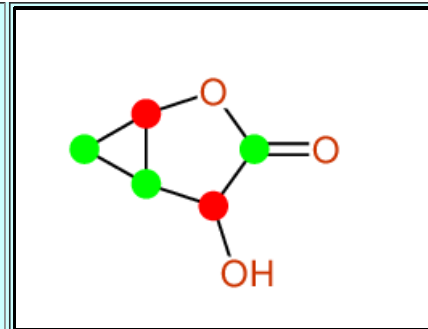
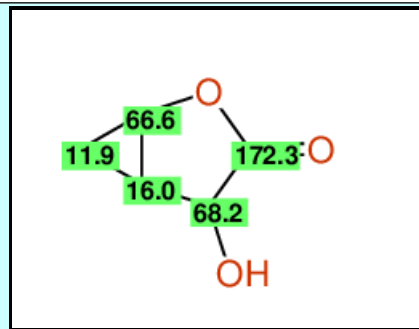
No line in reference: 



[Back to Complete Result](#)

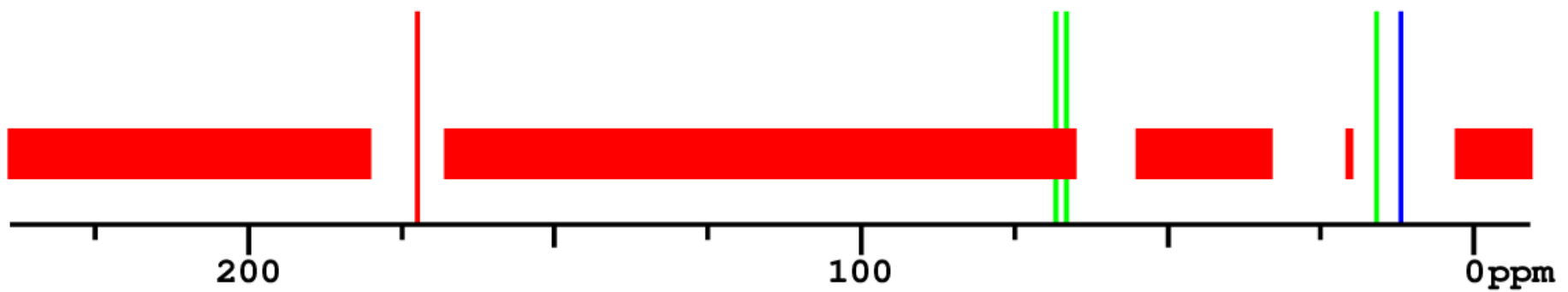
Structure Proposal #24

Structure	Similarity Measure
	<p>Deviation = 5.46 ppm Similarity = 60 % (Different pattern)</p> <p>$C_5H_6O_3$</p> <p>MWT = 114.06</p> <p>Search Web for this structure: YYNYNGRONAJGI</p>
Predicted Chemical Shiftvalues	Matching Map




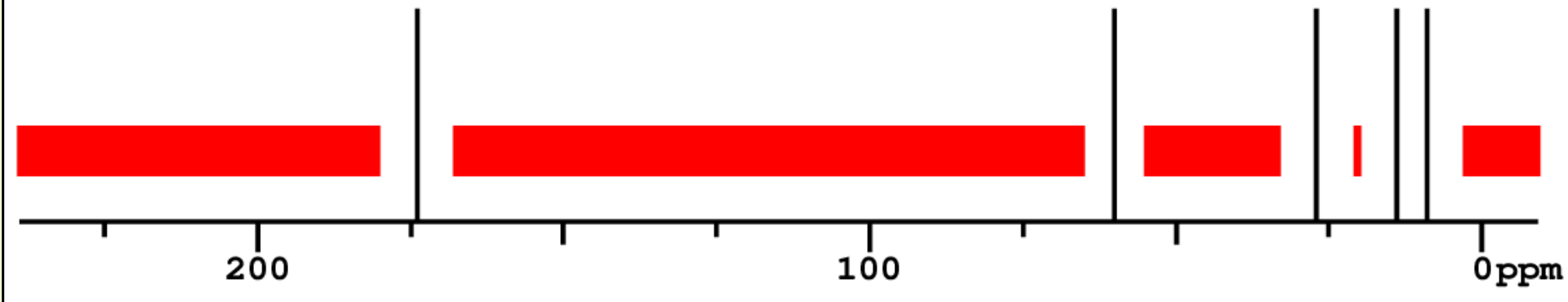
Predicted shift values

Signal multiplicity: S D T Q O E P ?



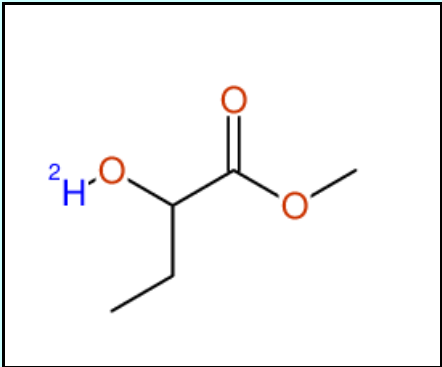
Experimental shift values

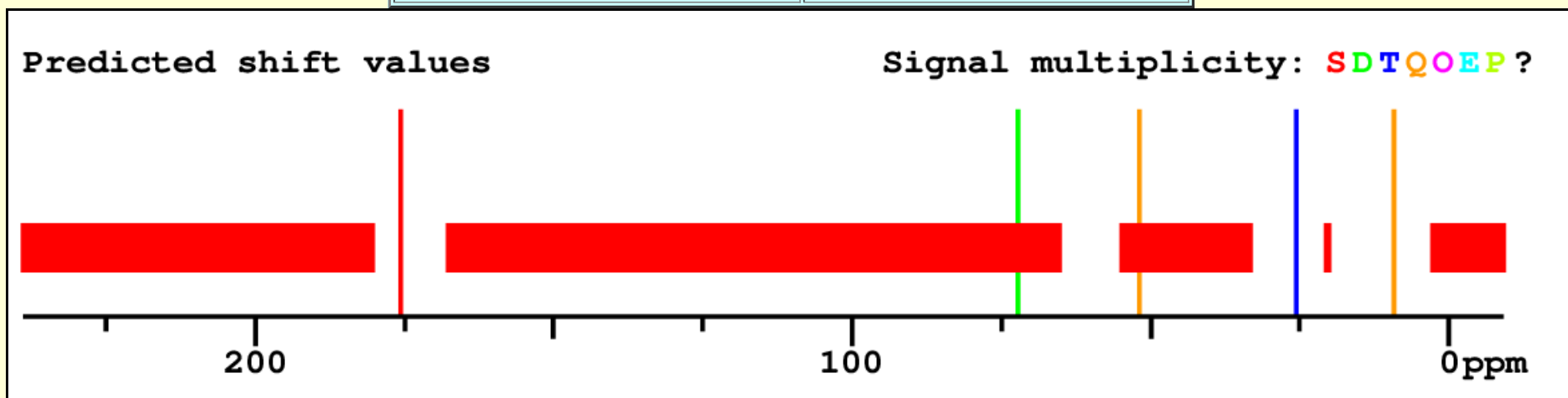
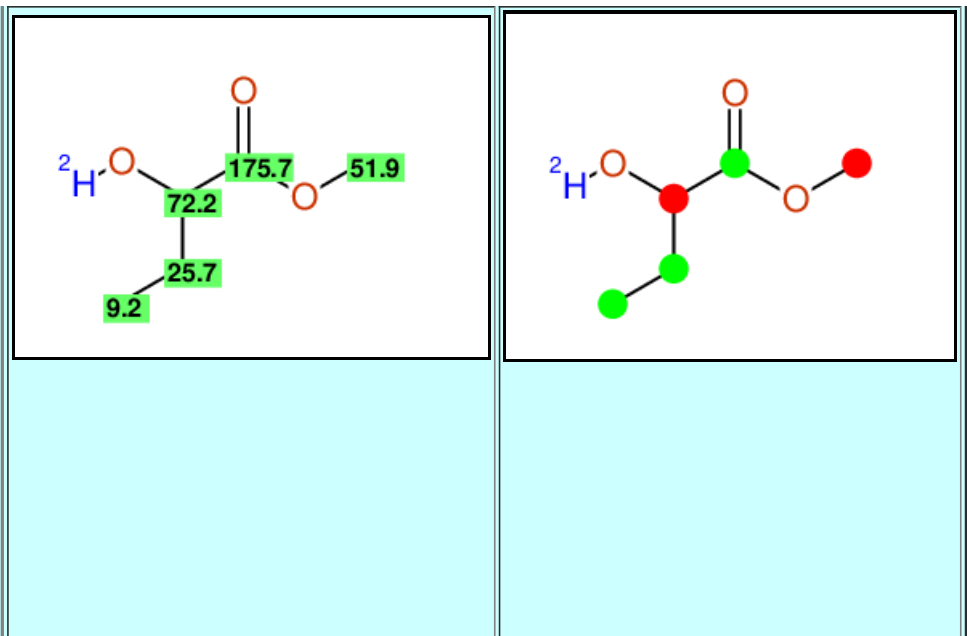
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[Back to Complete Result](#)

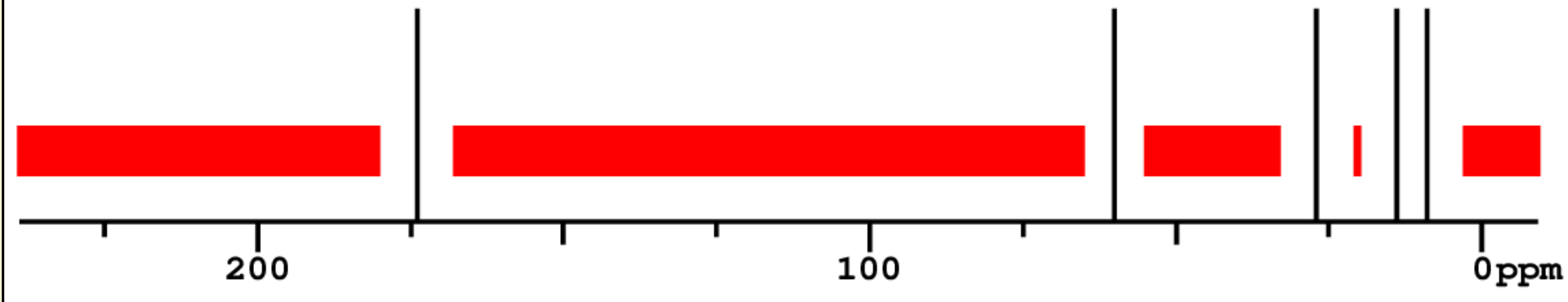
Structure Proposal #25

Structure	Similarity Measure
	<p>Deviation = 5.48 ppm Similarity = 60 % (Different pattern)</p> <p>$C_5H_{10}O_3$</p> <p>MWT = 119.06</p> <p>Search Web for this structure: DDMCDMDOHABRHD</p>
Predicted Chemical Shiftvalues	Matching Map



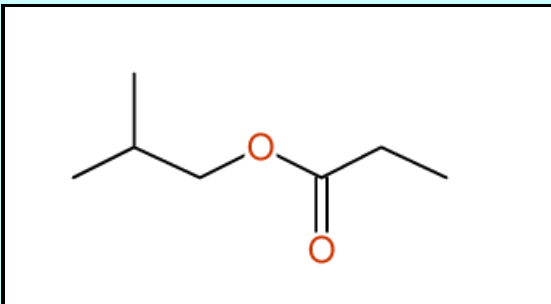
Experimental shift values

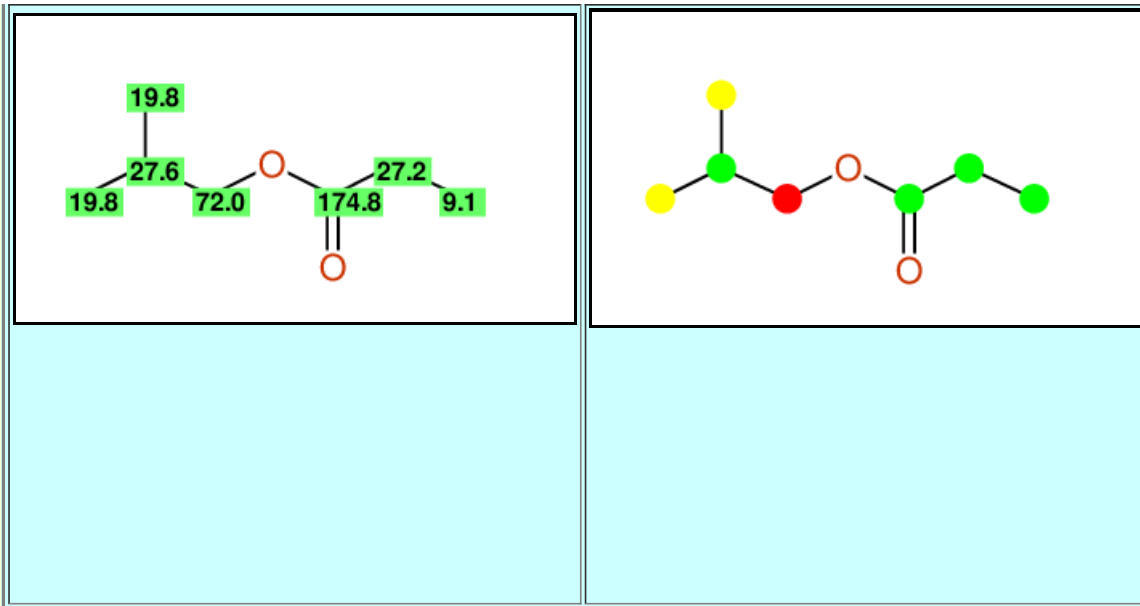
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[Back to Complete Result](#)

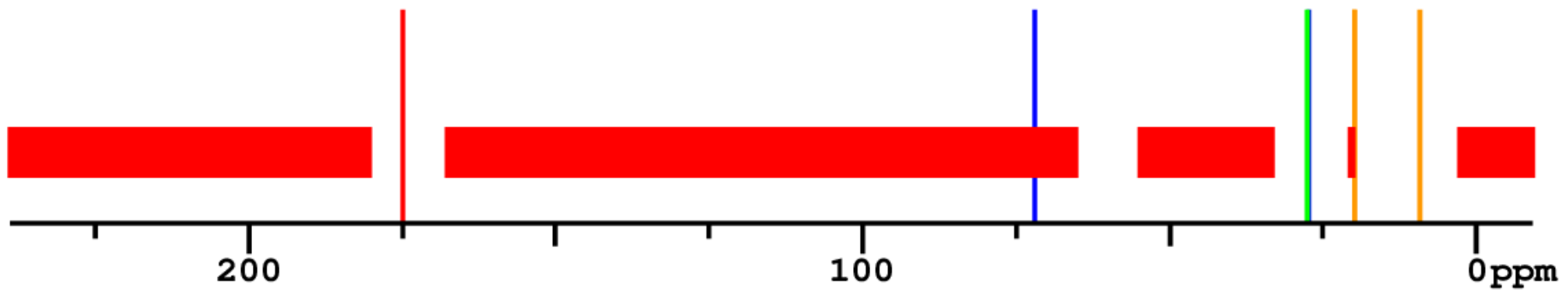
Structure Proposal #26

Structure	Similarity Measure
 <chem>CC(C)CCOC(=O)CC</chem>	<p>Deviation = 5.66 ppm Similarity = 71 % (Different pattern)</p> <p>C_7O_2</p> <p>MWT = 116.08</p> <p>Search Web for this structure: CPOGEOGDMOTURU</p>
Predicted Chemical Shiftvalues	Matching Map



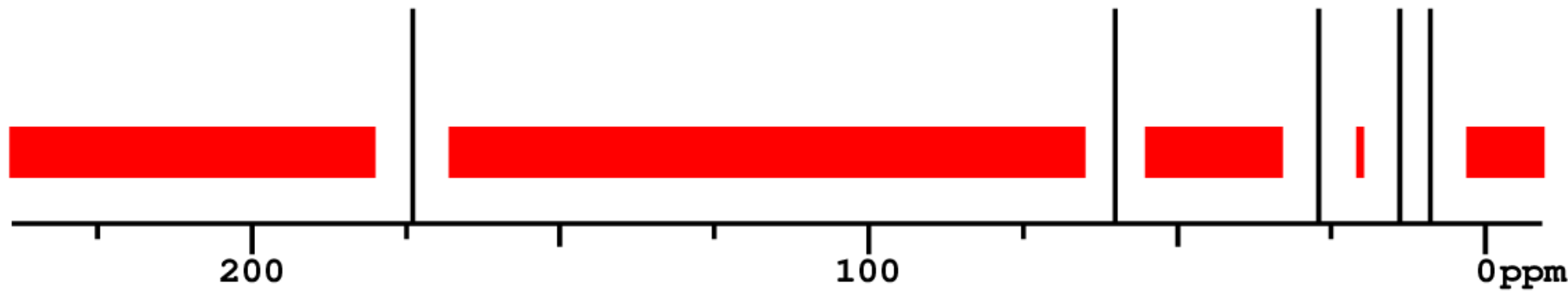
Predicted shift values

Signal multiplicity: S D T Q O E P ?



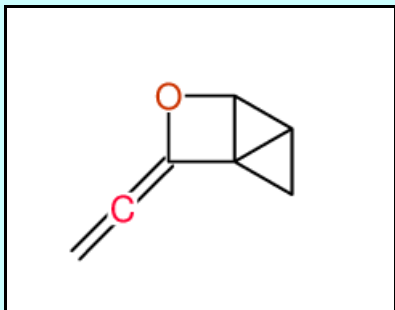
Experimental shift values

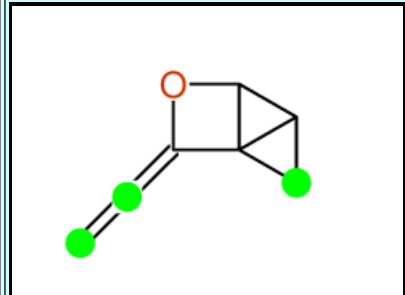
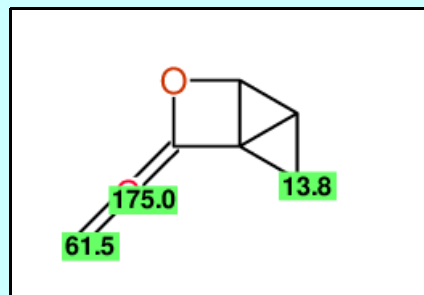
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[Back to Complete Result](#)

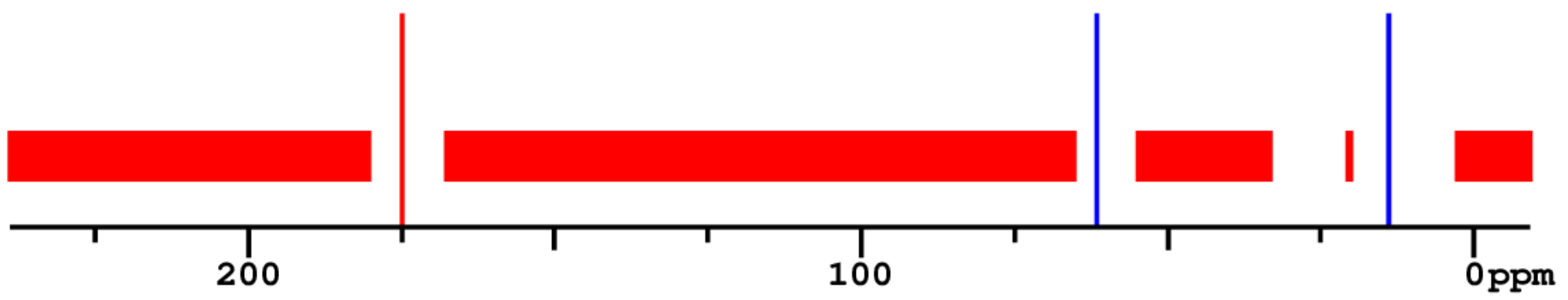
Structure Proposal #27

Structure	Similarity Measure
	Deviation = 5.83 ppm Similarity = 100 % C ₇ H ₆ O MWT = 106.08 Search Web for this structure: DCKHOMFWTGMJOV
Predicted Chemical Shiftvalues	Matching Map



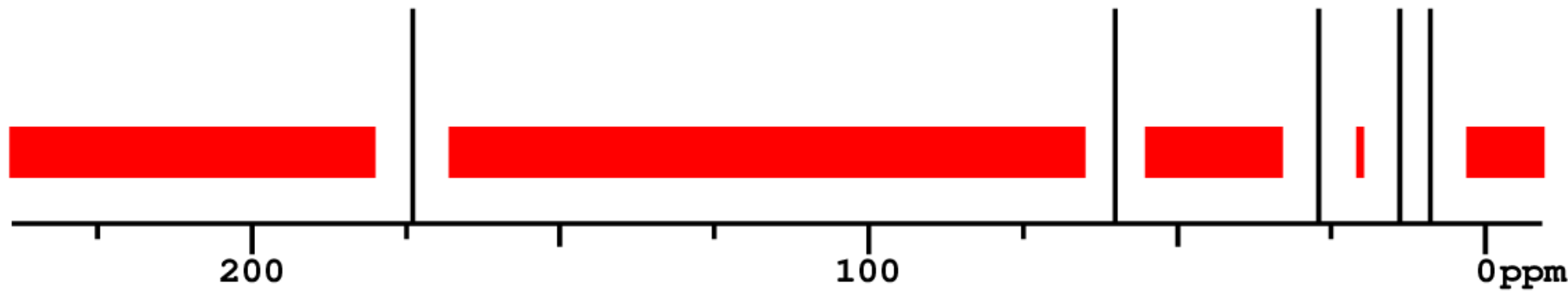
Predicted shift values

Signal multiplicity: S D T Q O E P ?



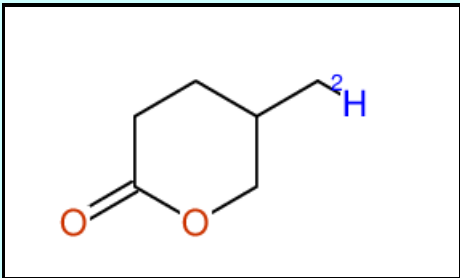
Experimental shift values

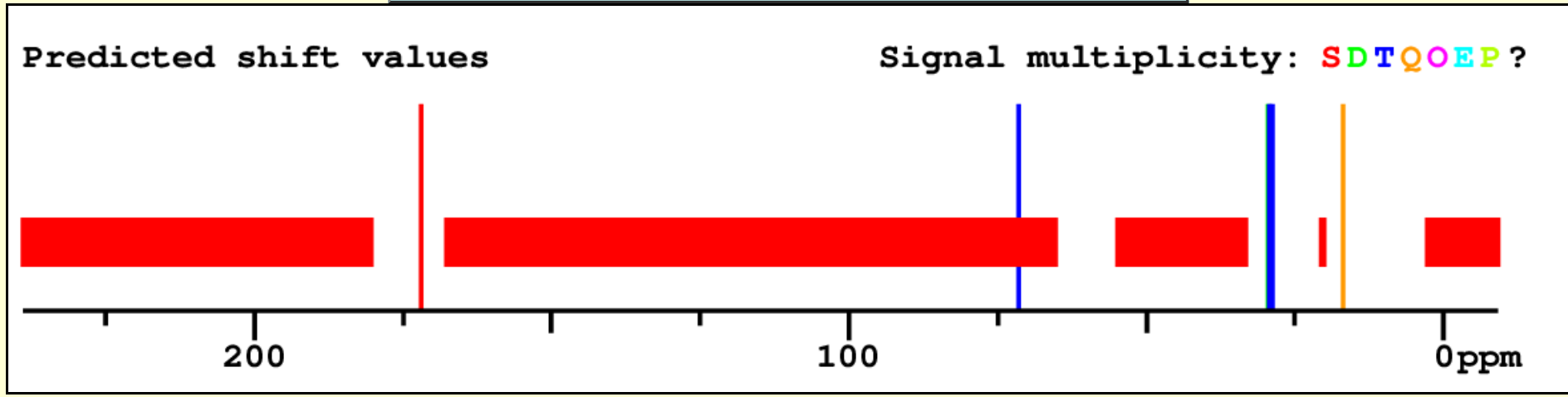
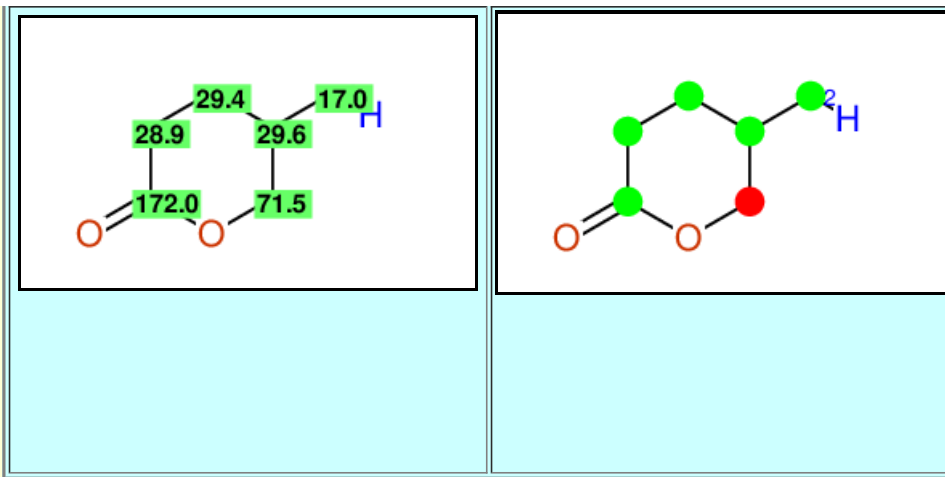
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[Back to Complete Result](#)

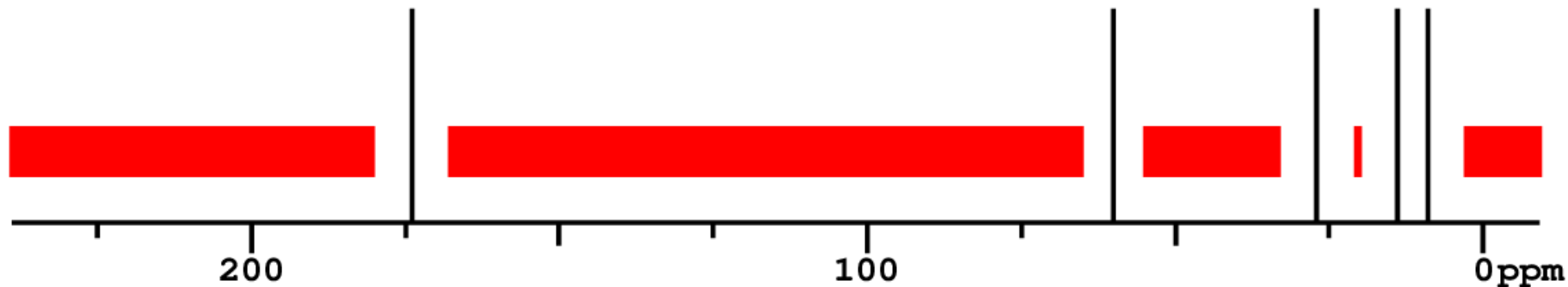
Structure Proposal #28

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



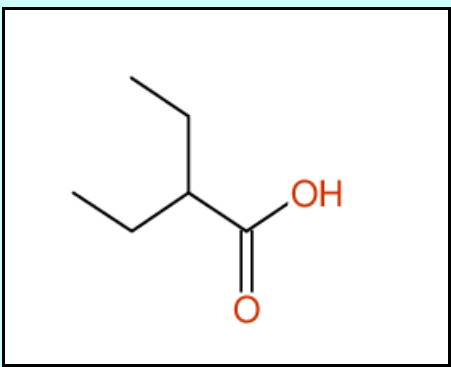
Experimental shift values

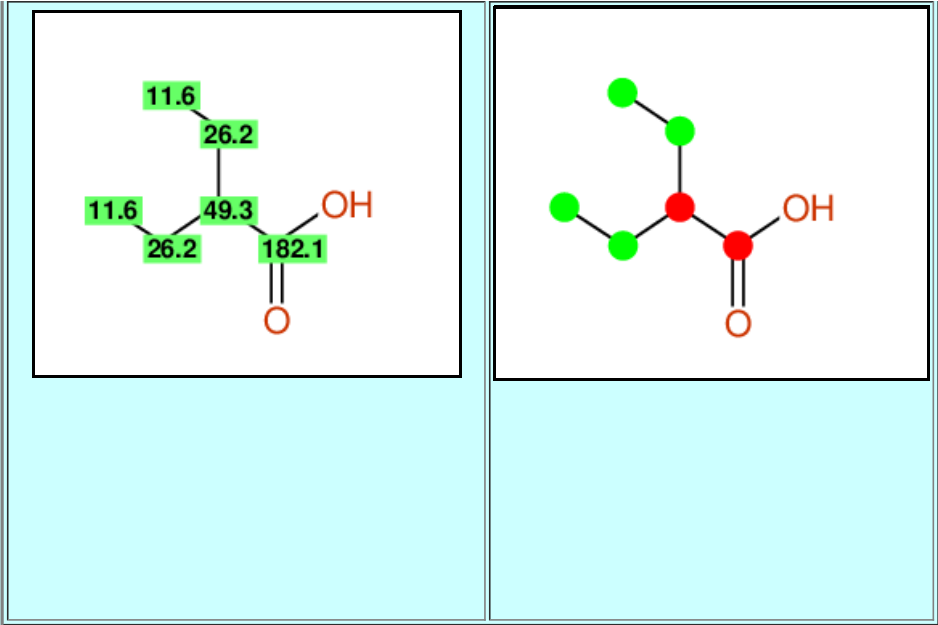
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[Back to Complete Result](#)

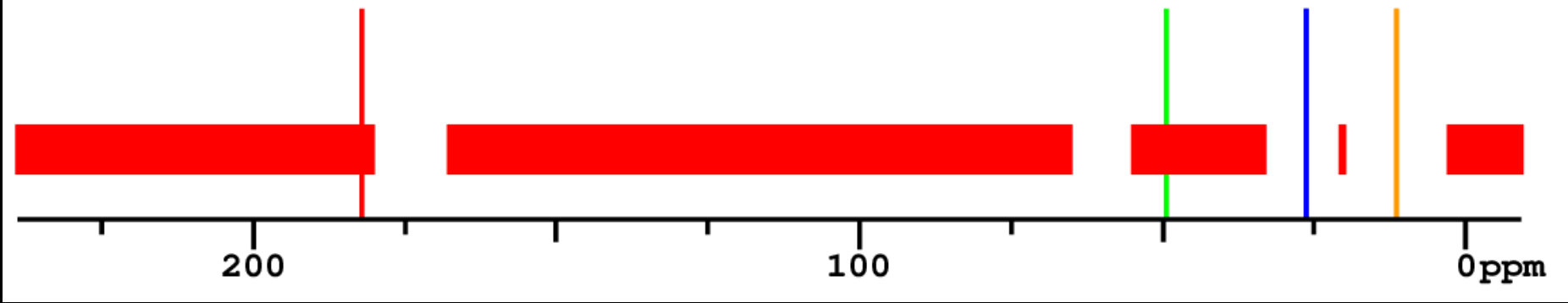
Structure Proposal #29

Structure	Similarity Measure
	<p>Deviation = 5.96 ppm Similarity = 67 % (Different pattern)</p> <p>C_6O_2</p> <p>MWT = 104.07</p> <p>Search Web for this structure: CUXRHJZMBXDZPJ</p>
Predicted Chemical Shiftvalues	Matching Map



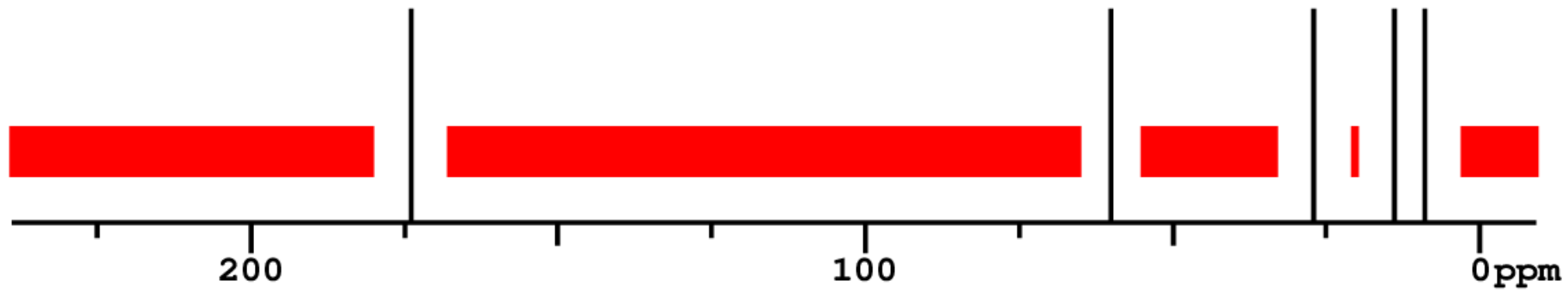
Predicted shift values

Signal multiplicity: S D T Q O E P ?



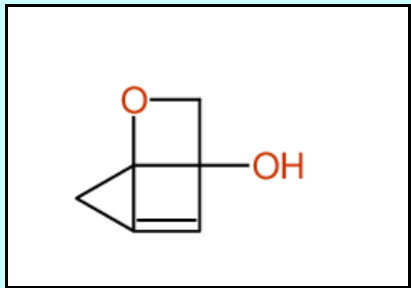
Experimental shift values

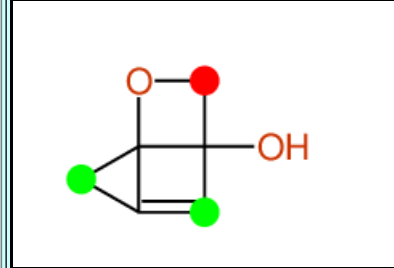
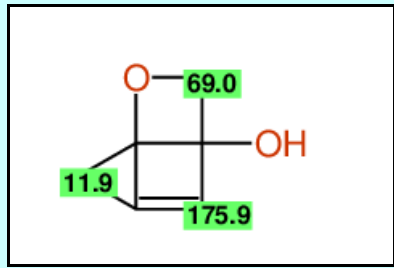
No line in reference: 



[Back to Complete Result](#)

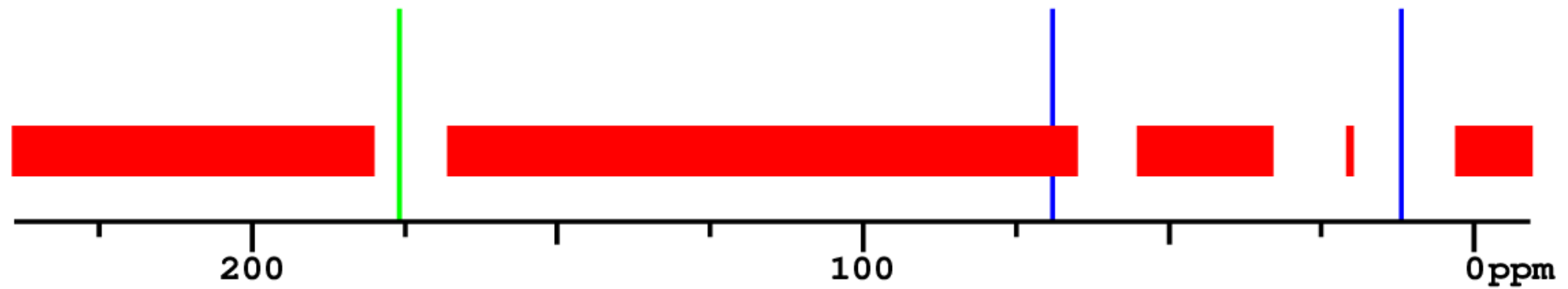
Structure Proposal #30

Structure	Similarity Measure
	<p>Deviation = 6.89 ppm Similarity = 67 % (Different pattern)</p> <p>$C_6H_6O_2$</p> <p>MWT = 110.07</p> <p>Search Web for this structure: INDSDELFJIPJJU</p>
Predicted Chemical Shiftvalues	Matching Map



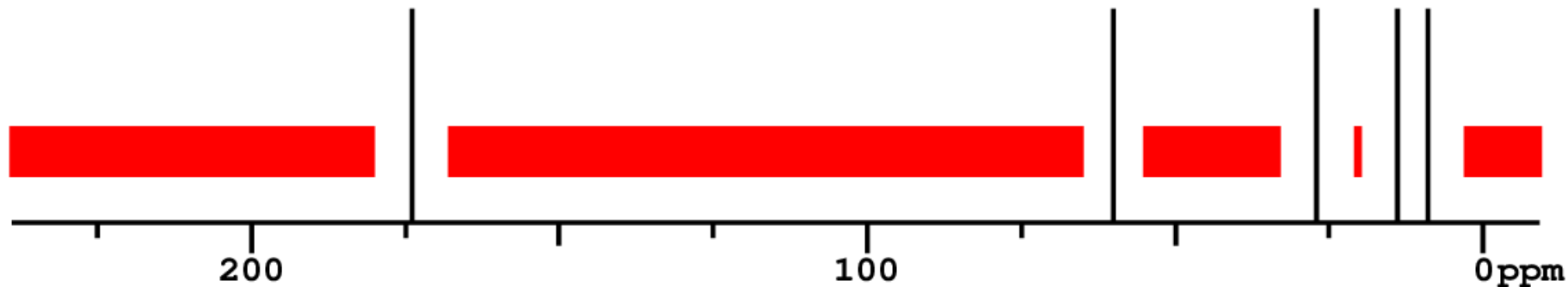
Predicted shift values

Signal multiplicity: S D T Q O E P ?



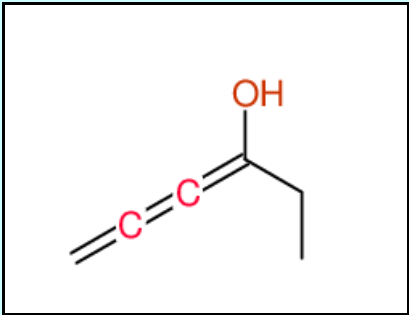
Experimental shift values

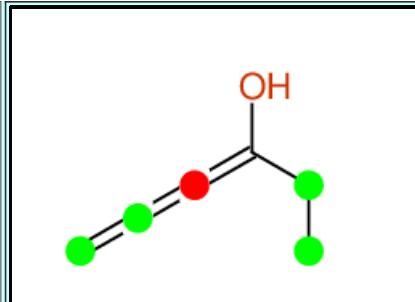
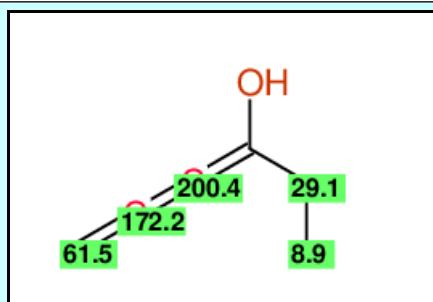
No line in reference: 



[Back to Complete Result](#)

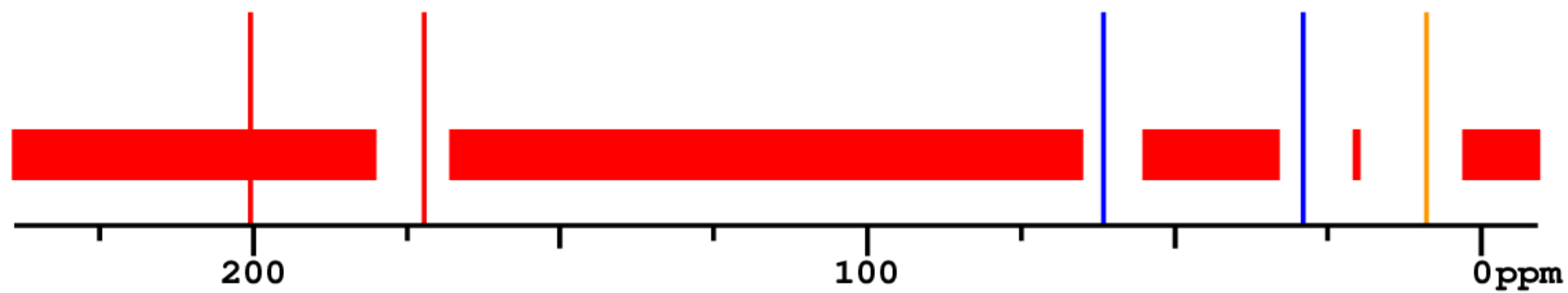
Structure Proposal #31

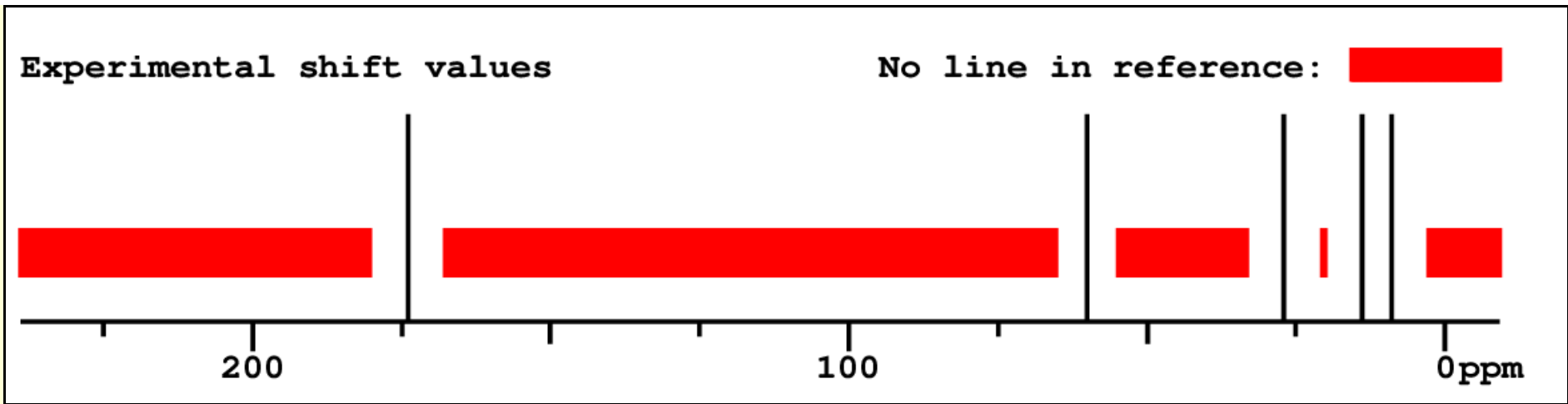
Structure	Similarity Measure
	<p>Deviation = 6.91 ppm Similarity = 80 % (Different pattern)</p> <p>C_6H_8O</p> <p>MWT = 96.07</p> <p>Search Web for this structure: XEXVNBAJTJGVQJ</p>
Predicted Chemical Shiftvalues	Matching Map



Predicted shift values

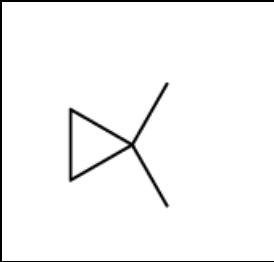
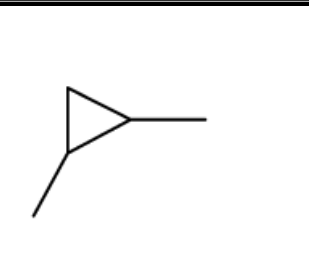
Signal multiplicity: **S** **D** **T** **Q** **O** **E** **P** ?





[Back to Complete Result](#)

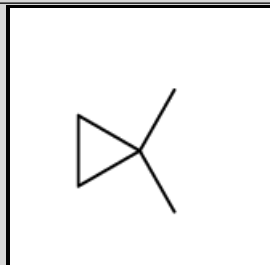
Summary of the 2 most frequently occurring parent ring systems
within the 4 best-fitting entries

<p>Occurrence: 1 in 4</p>			
<p>Occurrence: 1 in 4</p>			

Summary of the 10 most frequently occurring parent ring systems
within the 29 best-fitting entries

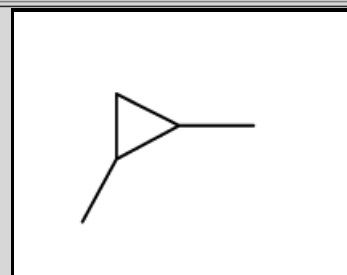
Occurrence:

1 in 29



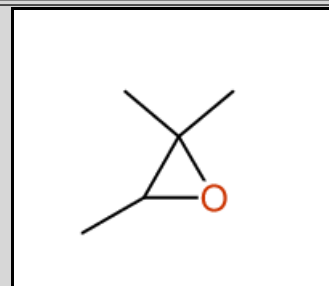
Occurrence:

1 in 29



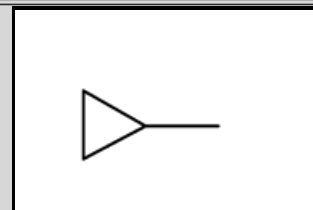
Occurrence:

1 in 29



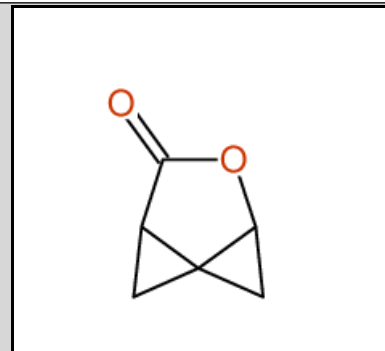
Occurrence:

1 in 29



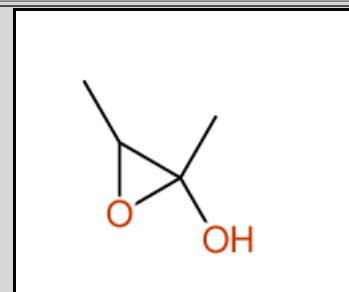
Occurrence:

1 in 29



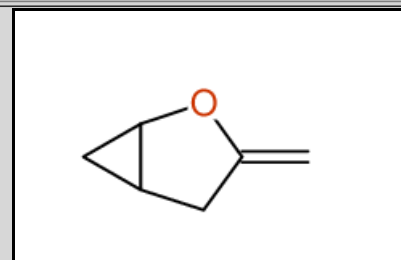
Occurrence:

1 in 29



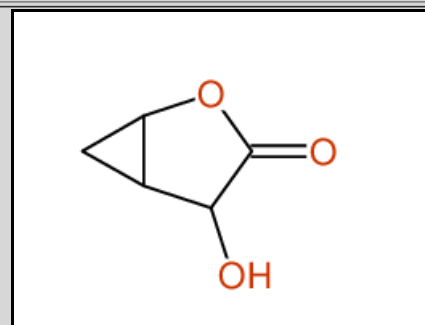
Occurrence:

1 in 29



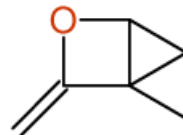
Occurrence:

1 in 29



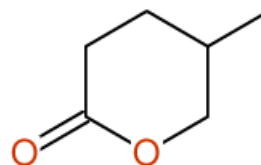
Occurrence:

1 in 29



Occurrence:

1 in 29



Summary of Processing

Checking existence of data and counting them:	144,833,798 entries in 3.142 seconds
Applying restraints from elemental composition:	7.692 seconds, 3,593,931 entries remain
Applying restraints from number of signals:	3.274 seconds, 104,807 entries remain
Searching 2,390,716,602 chemical shift values line-per-line:	39.617 seconds
Best 7,348 entries selected for analysis:	3.151 seconds
Ranking of 7,348 entries by similarity:	278.615 seconds
Deviation of best match:	2.21 ppm
Creating table and linking 7,348 structures to 475,803 INCHIKEY-pages:	1.074 seconds
Detailed Analysis of 31 structures including graphical representation:	9.257 seconds
Analysis of 29 structures for common parent ring systems:	0.012 seconds
Total CPU-usage:	347.438 seconds

Data transferred from disk:	1,723 MBytes out of 2,186,577 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 19:09 Page finished on 2021:05:19 at 19:23</p> <p>Have a nice day !</p>	