

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>

Automatic Resubmit:

Multiplicity omitted

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:09

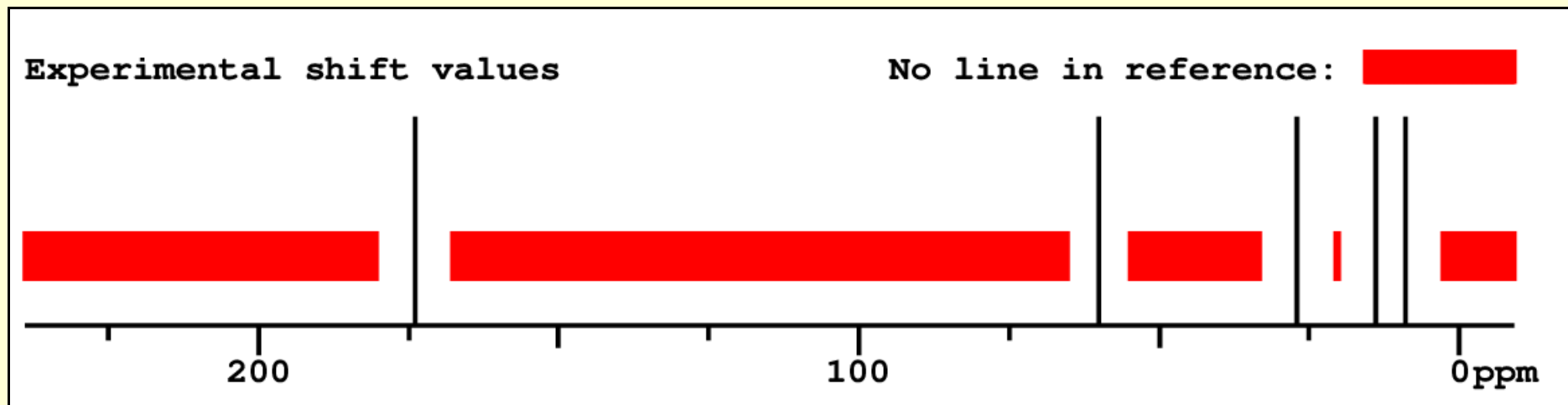
This page will be kept for 30 days here

<b>Name of Project:</b>	Test1
<b>Comment:</b>	Dereplication-engine
<b>Name of Compound:</b>	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 <sub>2</sub> or CH <sub>3</sub>	3.00
2	60.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	2.50
3	27.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00

4	14.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00
5	9.00	?	C or CH or CH <sub>2</sub> or CH <sub>3</sub>	3.00



<b>Additional Constraints given</b>	
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	

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

#### Elemental Composition of Reference Structures

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

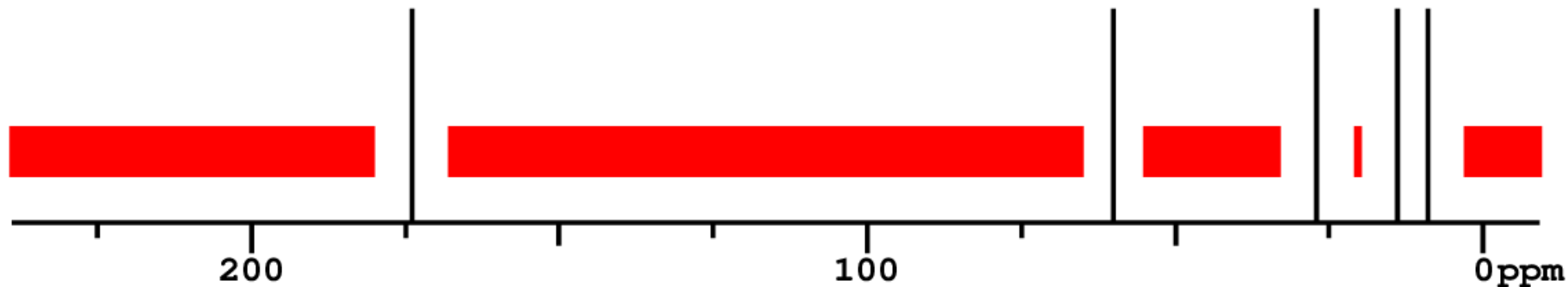
Available entries at each Screening-Step

<b>Total number of entries:</b>	<b>107,426,223</b>
<b>Applying requested elemental composition:</b>	<b>3,176,524 entries remain</b>
<b>Applying requested number of signals:</b>	<b>222,114 entries remain</b>

<b>Entries per line found out of 222,114 compounds</b>					
<b>Line number</b>	<b>Chemical Shift (ppm)</b>	<b>Multiplicity</b>	<b>Deviation (ppm)</b>	<b>Entries found</b>	<b>Evaluation result</b>
<b>1</b>	<b>174.00</b>	<b>?</b>	<b>3.00</b>	<b>33,015</b>	<b>Unspecific line</b>
<b>2</b>	<b>60.00</b>	<b>?</b>	<b>2.50</b>	<b>42,136</b>	<b>Unspecific line</b>
<b>3</b>	<b>27.00</b>	<b>?</b>	<b>3.00</b>	<b>84,656</b>	<b>Unspecific line</b>
<b>4</b>	<b>14.00</b>	<b>?</b>	<b>3.00</b>	<b>53,433</b>	<b>Unspecific line</b>
<b>5</b>	<b>9.00</b>	<b>?</b>	<b>3.00</b>	<b>30,057</b>	<b>Unspecific line</b>

Experimental shift values

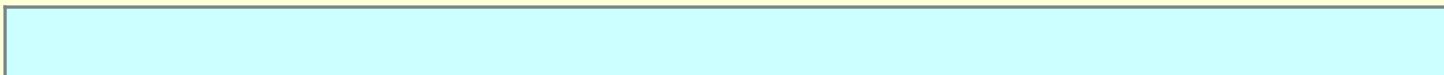
No line in reference: ██████████



Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	146	Selected for detailed analysis
4	2,048	Selected for detailed analysis
3	13,833	
2	49,148	
1	94,580	

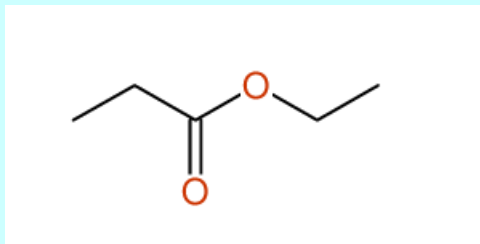
Best 17 Proposals shown for Compound: Propionic\_acid,ethylester::400MHz



0.87 -  
0.87ppm

3x found

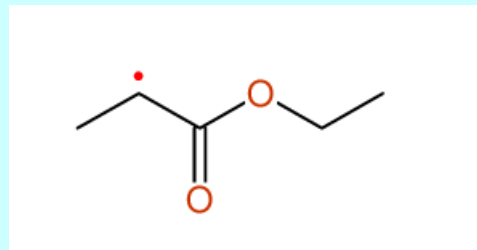
[FKRCODPIKNEYAC](#)



0.87 -  
0.87ppm

1x found

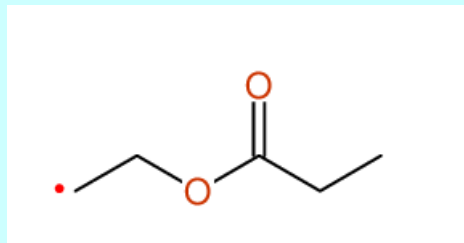
[UPLWNPAPKPCCE](#)



0.87 -  
0.87ppm

1x found

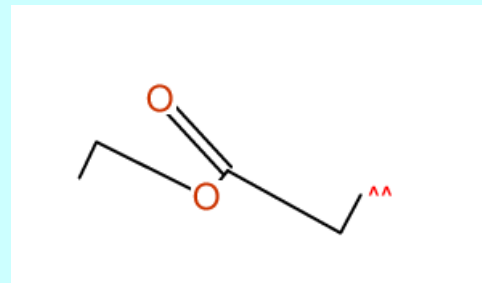
[IRGLFRDZYNBBCO](#)



0.87 -  
0.87ppm

1x found

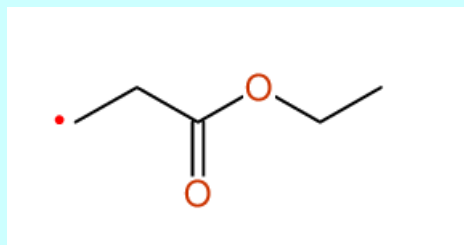
[BYLOWVUCDFUYIQ](#)



0.87 -  
0.87ppm

1x found

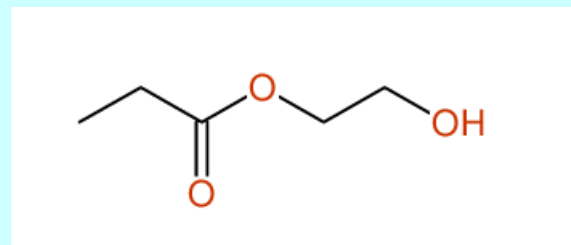
[SQKCNILPAQLIRC](#)



2.02 -  
2.02ppm

1x found

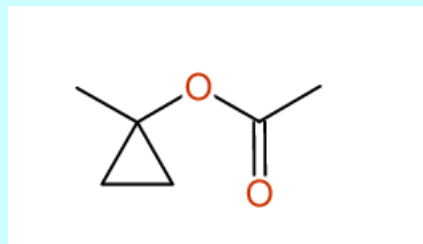
[SFAMKDPMPDEXGH](#)



2.45 -  
2.45ppm

1x found

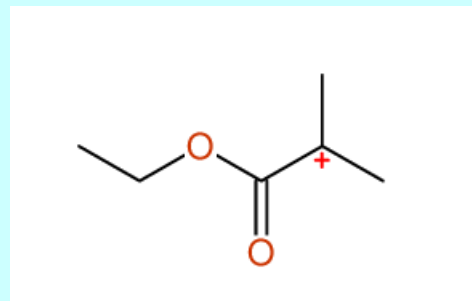
[MJRMRENRBUEGGM](#)



2.93 -  
2.93ppm

1x found

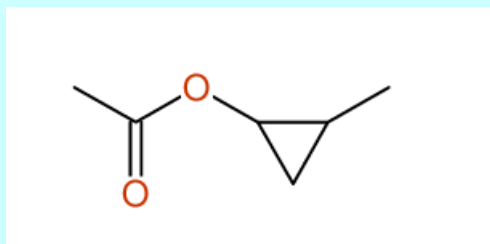
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2.95 -  
2.95ppm

1x found

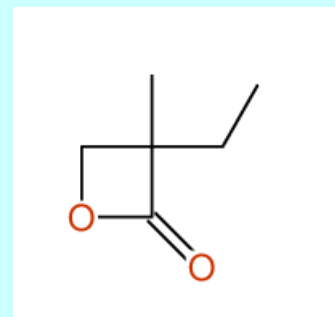
[OTXJUSAVQLCSFT](#)



4.17 -  
4.17ppm

1x found

[UFTRVHTYHBMWOF](#)

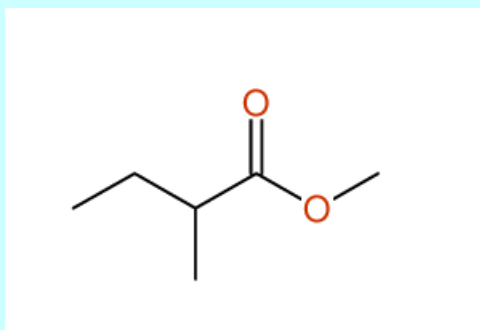




5.25 -  
5.25ppm

1x found

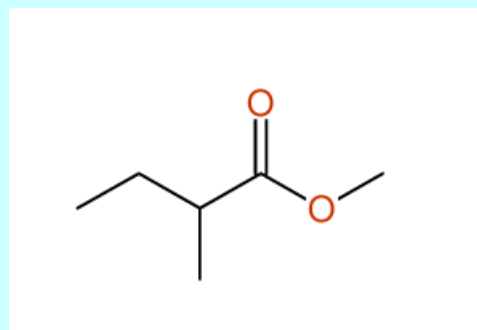
[YMRCZGBILKTSL](#)



5.25 -  
5.25ppm

1x found

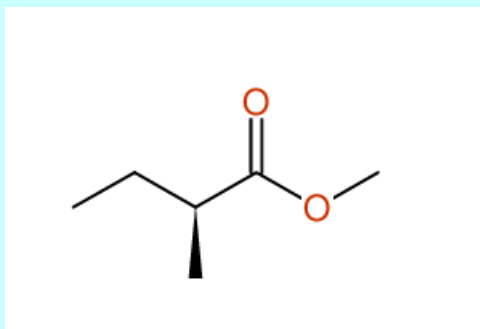
[OYGDMLWOJBKWLN](#)



5.25 -  
5.25ppm

4x found

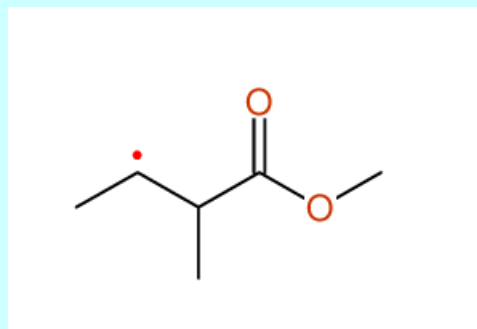
[OCWLYWIFENDCWRZ](#)



5.25 -  
5.25ppm

1x found

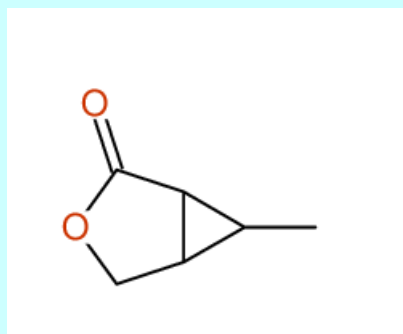
[WKWGMFVUDZAZEV](#)



5.38 -  
5.38ppm

1x found

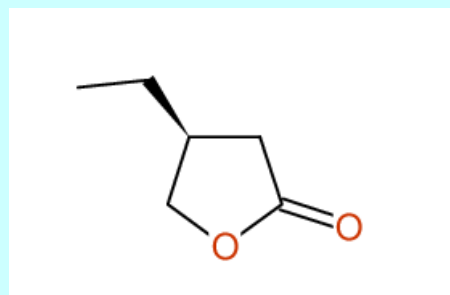
[ODZSNSOKRZBPDY](#)



6.77 -  
6.88ppm

3x found

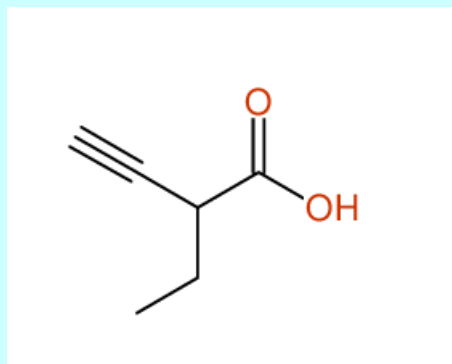
[MDQZVJSUBKPTHG](#)



8.49 -  
8.49ppm

1x found

[YHXLBJJLZTWBAZ](#)



2,194 [Structure proposals](#) found for your C-NMR Spectrum

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

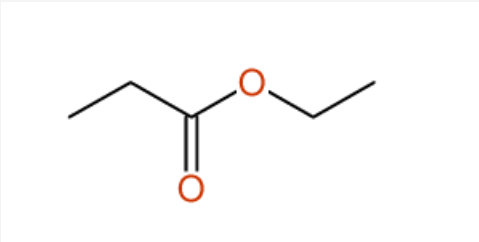

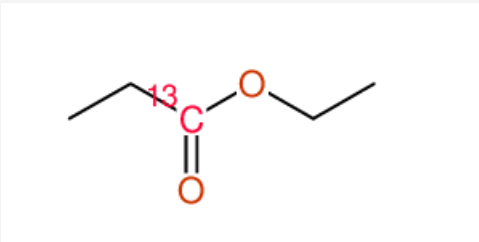

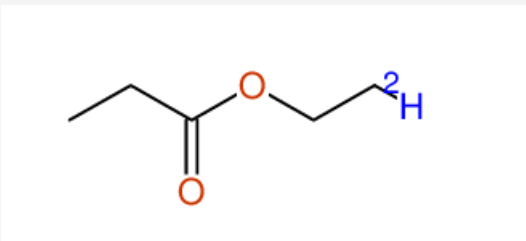

Similarity  
(ppm) ▲▼

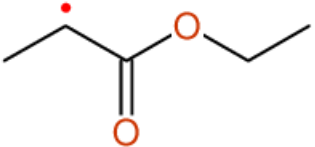
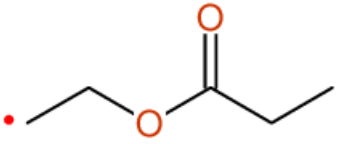
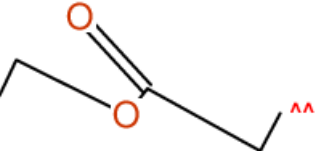
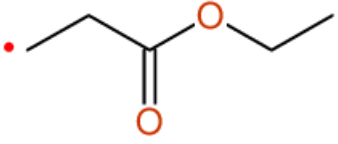
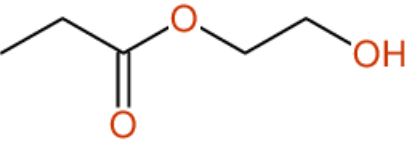
Structure Diagram

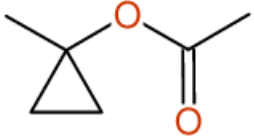
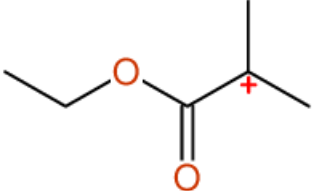
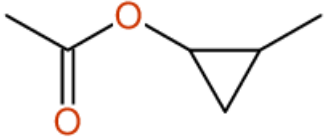
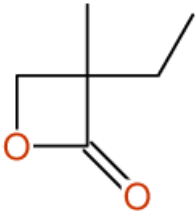
Molecular Formula  
Molecular Weight ▲▼

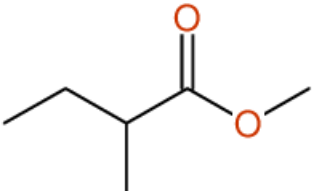
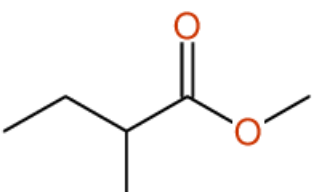
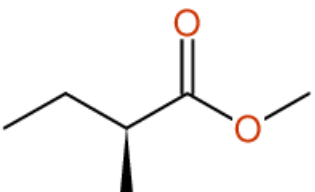

InChIkey

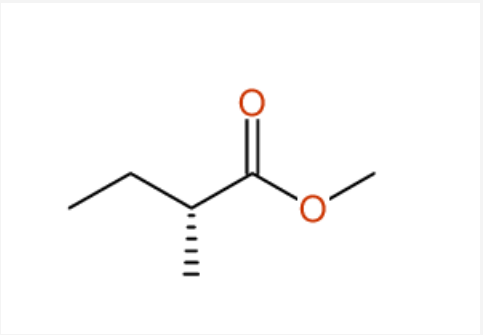

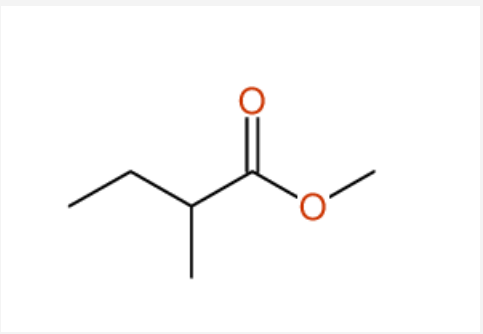

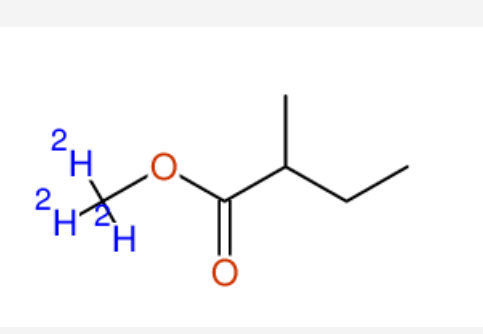

Experimental Data  
in CSEARCH ▲▼

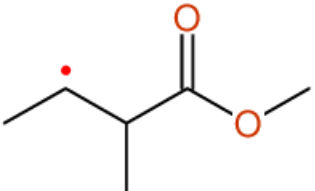
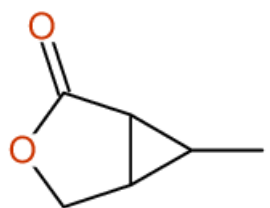
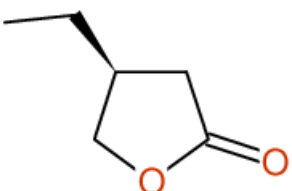

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #1</p> <p>0.87</p> <p><a href="#">Details</a></p>		<p><math>C_5H_{10}O_2</math></p> <p>MWT = 102.055</p>	<p>Proposal #1</p> <p>Structure-ID: 2,881,257</p> <p><a href="#">FKRCODPIKNYEAC-UHFFFAOYAW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

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<b>Proposal #4</b>  0.87 <a href="#">Details</a>		$C_5H_{10}O_2$ MWT = 101.055	Proposal #4 Structure-ID: 18,145,214 <a href="#">UPRLWNPAOPKPCE-UHFFFAOYAG</a>	
<b>Proposal #5</b>  0.87 <a href="#">Details</a>		$C_5H_{10}O_2$ MWT = 101.055	Proposal #5 Structure-ID: 19,005,681 <a href="#">IRGLFRDZYNBBCO-UHFFFAOYAO</a>	
<b>Proposal #6</b>  0.87 <a href="#">Details</a>		$C_5H_{10}O_2$ MWT = 100.055	Proposal #6 Structure-ID: 26,212,372 <a href="#">BYLOWVUCDFUYIQ-UHFFFAOYAU</a>	
<b>Proposal #7</b>  0.87 <a href="#">Details</a>		$C_5H_{10}O_2$ MWT = 101.055	Proposal #7 Structure-ID: 3,764,581 <a href="#">SQKCNILPAQLIRC-UHFFFAOYAO</a>	
<b>Proposal #8</b>  2.02 <a href="#">Details</a>		$C_5H_{10}O_3$ MWT = 118.055	Proposal #8 Structure-ID: 4,551,455 <a href="#">SFAMKDPMPDEXGH-UHFFFAOYAK</a>	

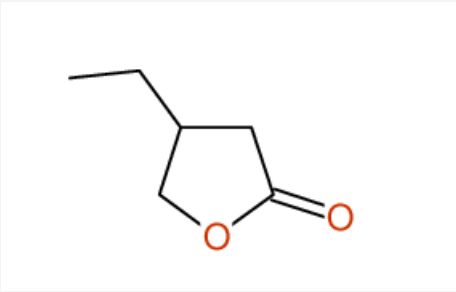

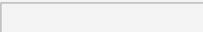

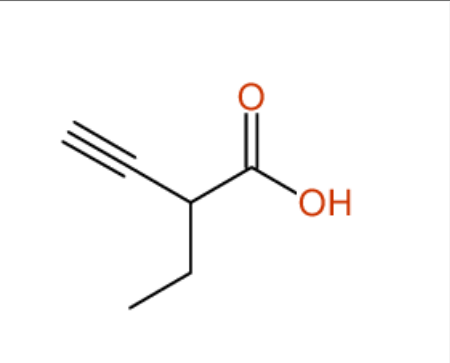
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<b>Proposal #9</b>  2.45  <a href="#">Details</a>		$C_6H_{10}O_2$ MWT = 114.066	Proposal #9 Structure-ID: 4,761,573 <a href="#">MJRMRENRBUDEGM-UHFFFAOYAU</a>	
<b>Proposal #10</b>  2.93  <a href="#">Details</a>		$C_6H_{11}O_2$ MWT = 115.066	Proposal #10 Structure-ID: 102,709,334 <a href="#">BNJCQKCNZHKCSF-UHFFFAOYAU</a>	
<b>Proposal #11</b>  2.95  <a href="#">Details</a>		$C_6H_{10}O_2$ MWT = 114.066	Proposal #11 Structure-ID: 59,447,594 <a href="#">OTXJUSAVQLCSFT-UHFFFAOYAM</a>	
<b>Proposal #12</b>  4.17  <a href="#">Details</a>  Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #12 Structure-ID: 3,924,833 <a href="#">UFTRVHTYHBMWOF-UHFFFAOYAW</a>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #13  5.25  <a href="#">Details</a>  Different pattern		$C_6H_{10}O_2$  MWT = 114.066	Proposal #13  Structure-ID: 55,101,808  <a href="#">YMRCZGBILKTSCl-UHFFFAOYAH</a>	
Proposal #14  5.25  <a href="#">Details</a>  Different pattern		$C_6H_{10}O_2$  MWT = 114.066	Proposal #14  Structure-ID: 57,060,396  <a href="#">OYGDMLWOJBKWLN-UHFFFAOYAV</a>	
Proposal #15  5.25  <a href="#">Details</a>  Different pattern		$C_6H_{12}O_2$  MWT = 116.066	Proposal #15  Structure-ID: 4,634,567  <a href="#">OCWLYWIFNDCWRZ-YFKPBYRVBR</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH  

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #16</p> <p>5.25</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.066</p>	<p>Proposal #16</p> <p>Structure-ID: 4,635,625</p> <p><a href="#">OCWLYWIFNDCWRZ-RXMQYKEDBJ</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #17</p> <p>5.25</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.066</p>	<p>Proposal #17</p> <p>Structure-ID: 2,886,286</p> <p><a href="#">OCWLYWIFNDCWRZ-UHFFFAOYAL</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 
<p>Proposal #18</p> <p>5.25</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{12}O_2</math></p> <p>MWT = 119.066</p>	<p>Proposal #18</p> <p>Structure-ID: 57,309,465</p> <p><a href="#">OCWLYWIFNDCWRZ-HPRDVNIFEY</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 

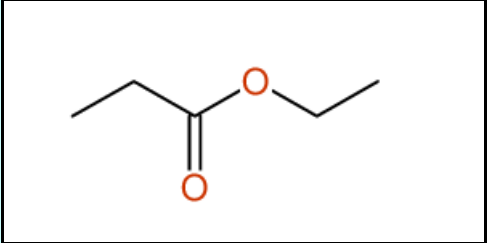
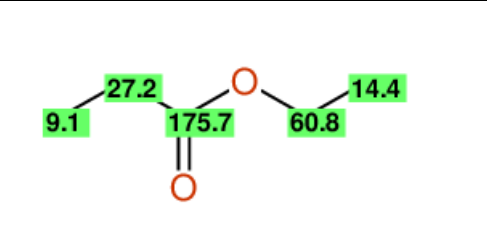
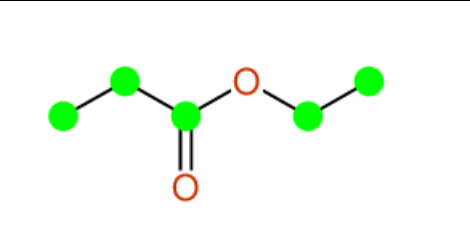
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #19</p> <p>5.25</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{11}O_2</math></p> <p>MWT = 115.066</p>	<p>Proposal #19</p> <p>Structure-ID: 106,235,255</p> <p><a href="#">WKWGMFVUDZAZEV-UHFFFAOYAX</a></p>	
<p>Proposal #20</p> <p>5.38</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_8O_2</math></p> <p>MWT = 112.066</p>	<p>Proposal #20</p> <p>Structure-ID: 24,501,304</p> <p><a href="#">ODZSNSOKRZBPDY-UHFFFAOYAR</a></p>	
<p>Proposal #21</p> <p>6.77</p> <p><a href="#">Details</a></p> <p>Different pattern</p>		<p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.066</p>	<p>Proposal #21</p> <p>Structure-ID: 51,765,446</p> <p><a href="#">MDQZVJSUBKPTHG-YFKPBYRVBH</a></p>	<p>Availability of <a href="#">NMR-Data</a> in CSEARCH</p> 



Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #22  6.88  <a href="#">Details</a>  Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #22 Structure-ID: 2,898,486 <a href="#">MDQZVJSUBKPTHG-UHFFFAOYAB</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH 
Proposal #23  6.88  <a href="#">Details</a>  Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #23 Structure-ID: 58,560,087 <a href="#">MDQZVJSUBKPTHG-RXMQYKEDBZ</a>	Availability of <a href="#">NMR-Data</a> in CSEARCH 
Proposal #24  8.49  <a href="#">Details</a>  Different pattern		$C_6H_8O_2$ MWT = 112.066	Proposal #24 Structure-ID: 3,751,880 <a href="#">YHXLBJJLZTWBAZ-UHFFFAOYAE</a>	

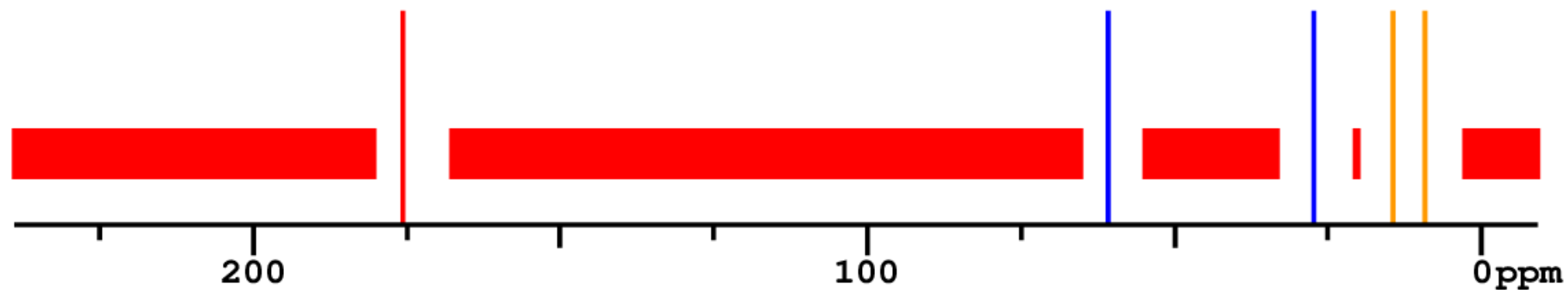
### Detailed Analysis

## 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: <a href="#">FKRCODPIKNYEAC</a>  <a href="#">Availability</a>
Predicted Chemical Shiftvalues	Matching Map
	

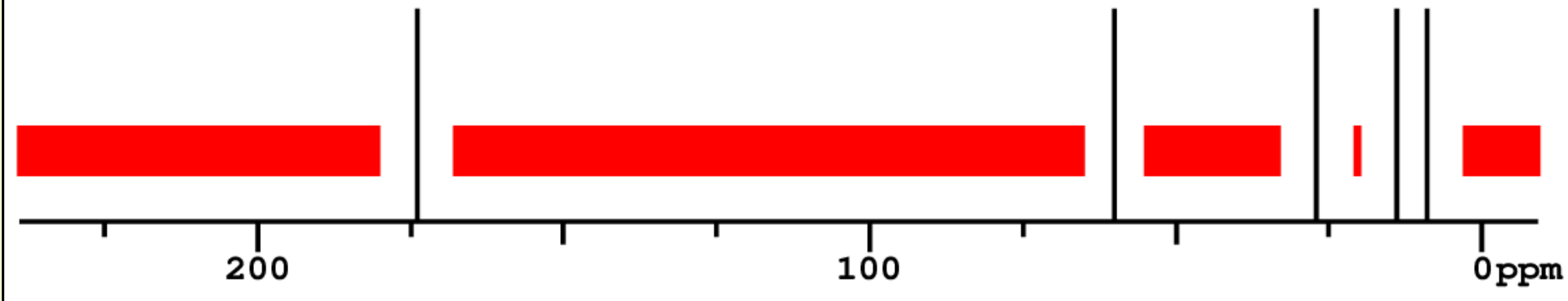
Predicted shift values

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



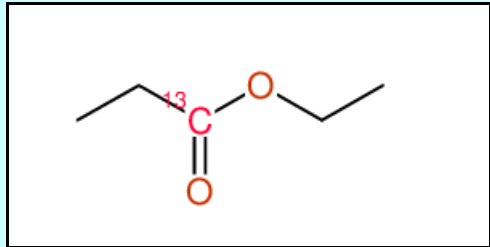
Experimental shift values

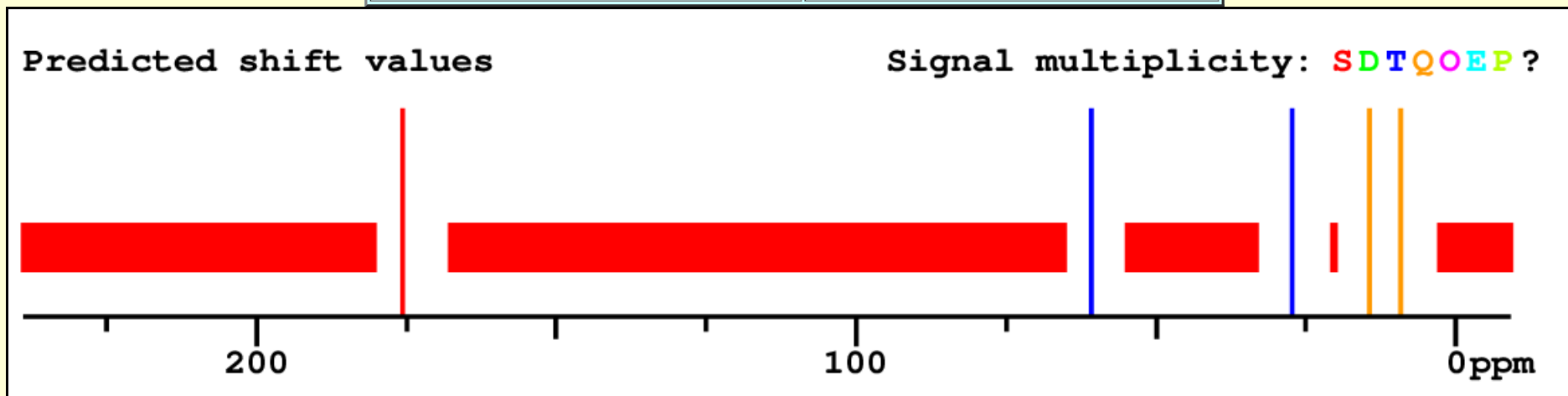
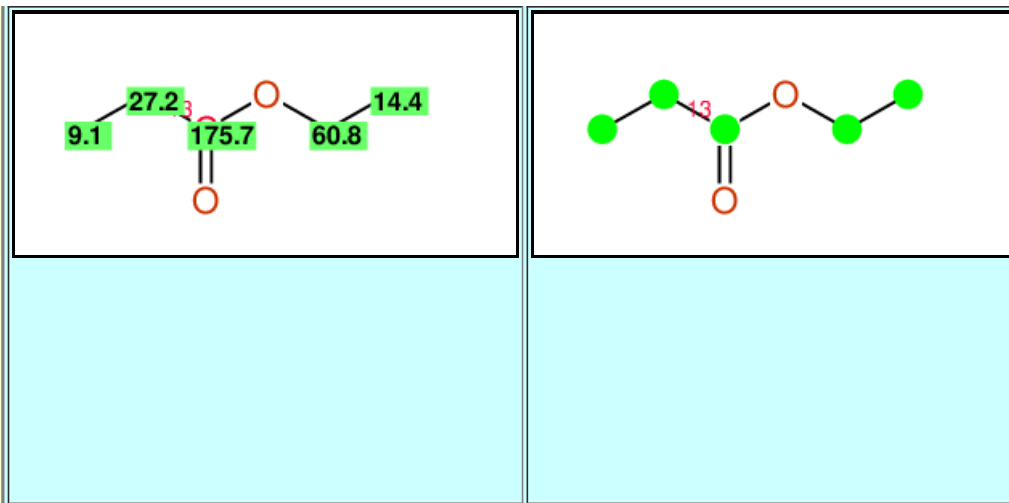
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[Back to Complete Result](#)

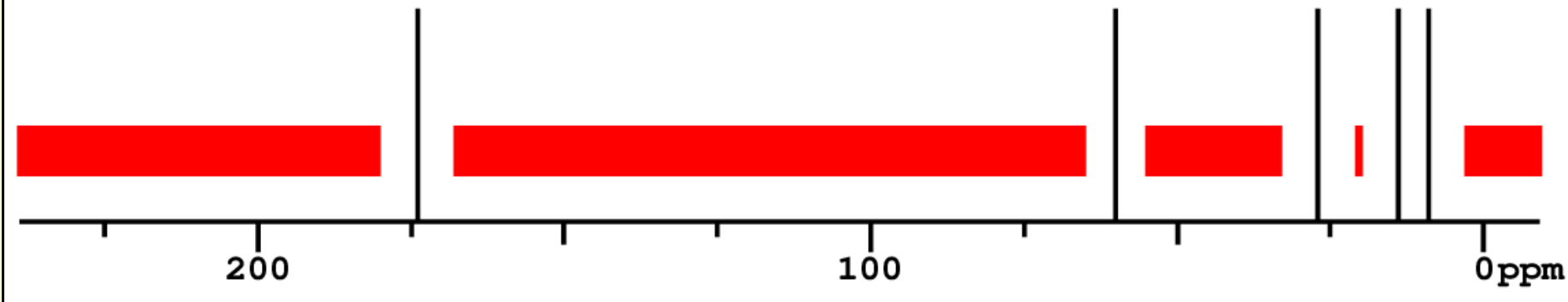
### Structure Proposal #2

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



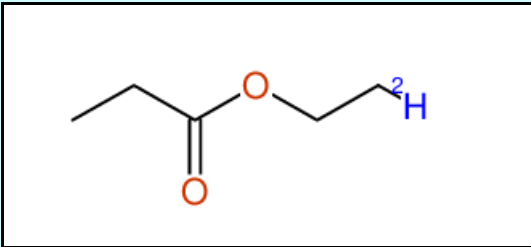
Experimental shift values

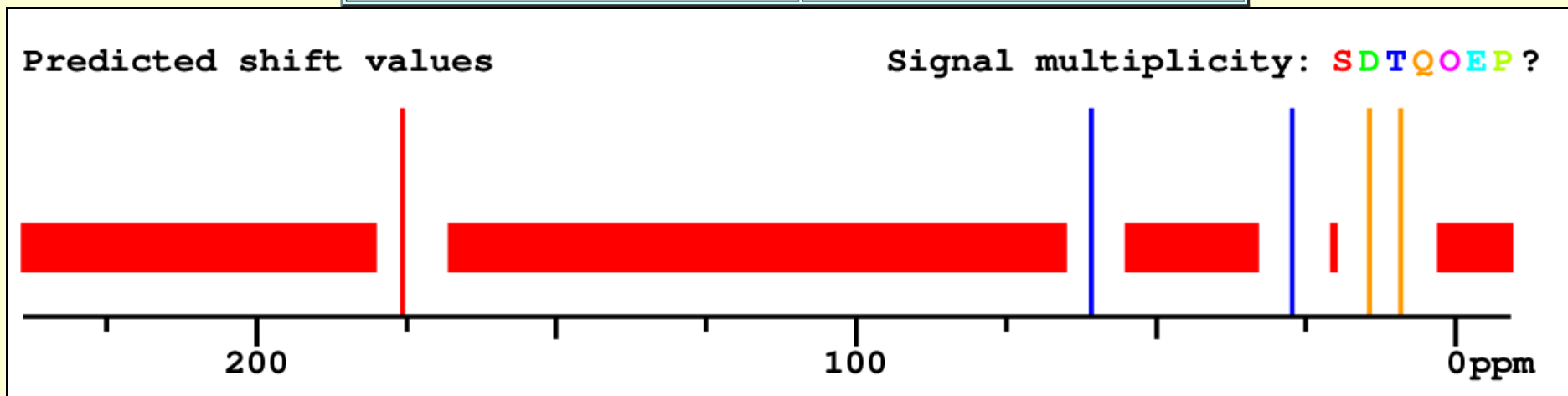
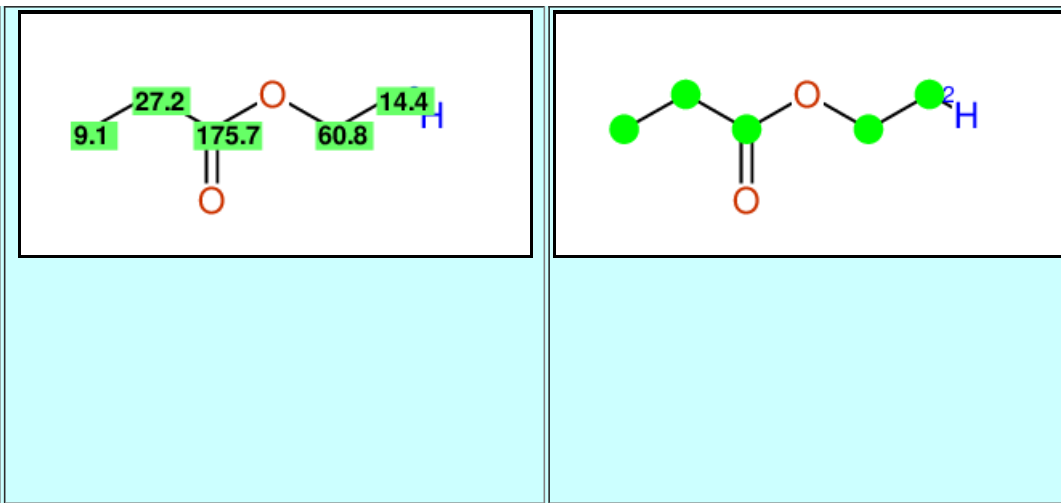
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[Back to Complete Result](#)

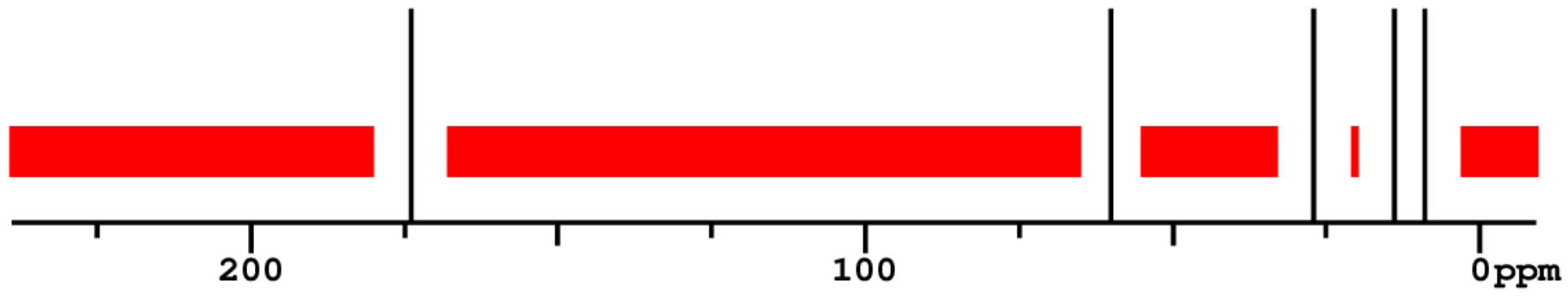
### Structure Proposal #3

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



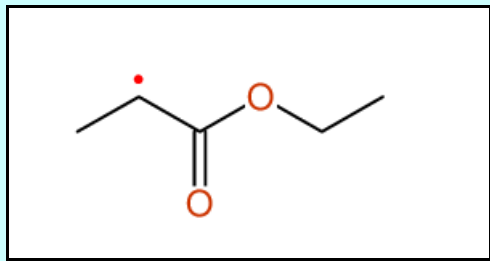
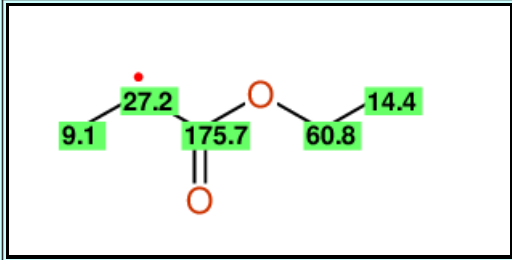
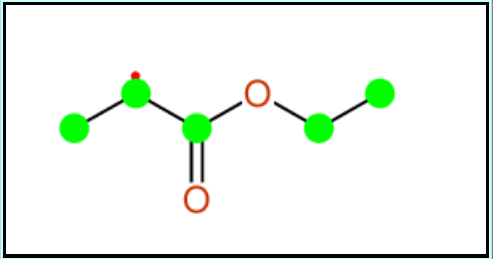
Experimental shift values

No line in reference: 



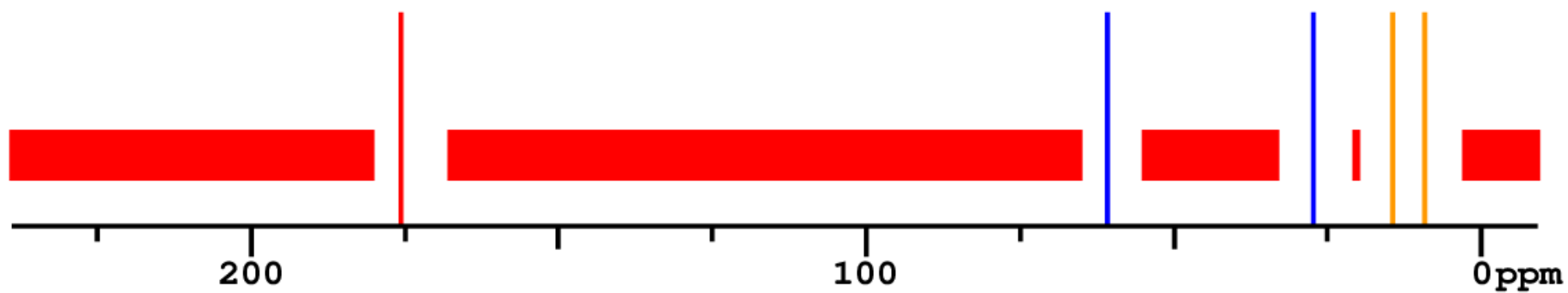
[Back to Complete Result](#)

#### Structure Proposal #4

Structure	Similarity Measure
	Deviation = 0.87 ppm Similarity = 100 %  C <sub>5</sub> H <sub>9</sub> O <sub>2</sub>  MWT = 101.06  Search Web for this structure: <a href="#">UPRLWNPAOPKPCE</a>
Predicted Chemical Shiftvalues	Matching Map
	

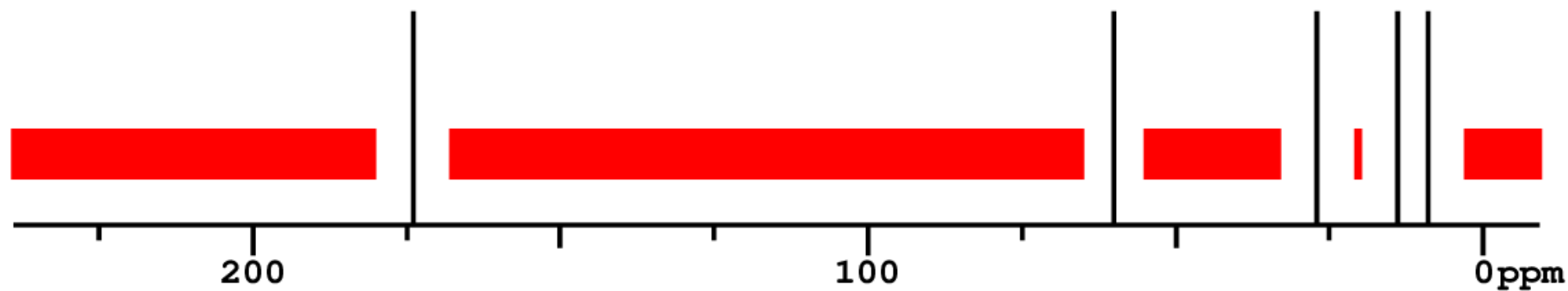
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]

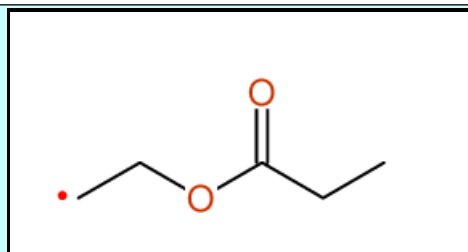


[Back to Complete Result](#)

### Structure Proposal #5

Structure	Similarity Measure

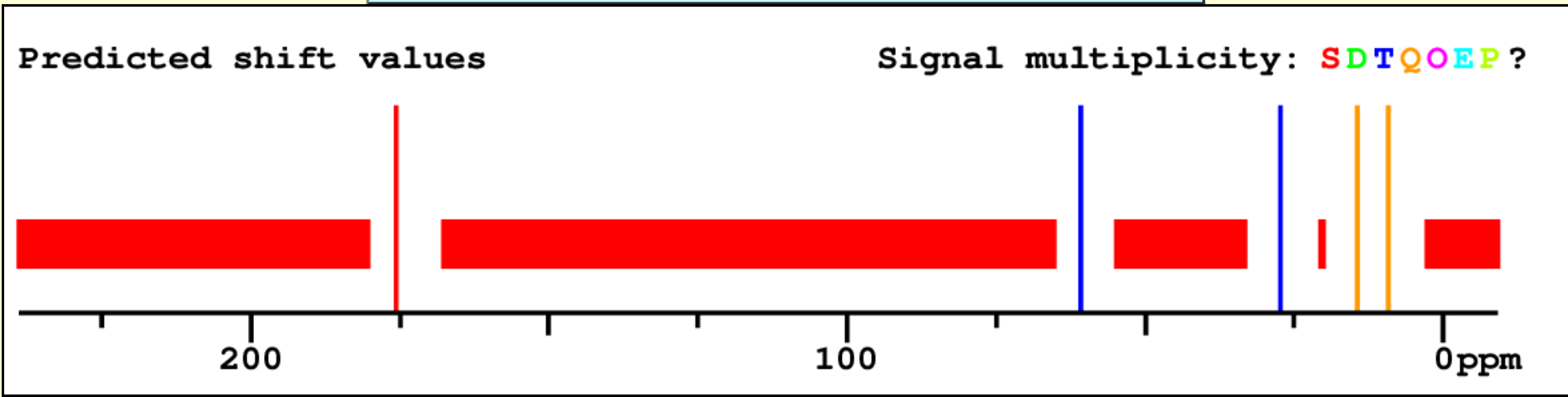
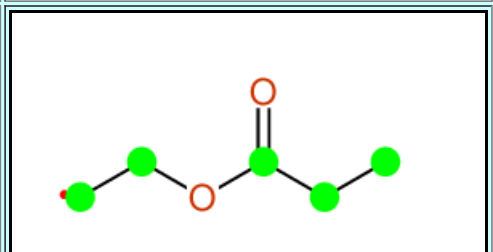
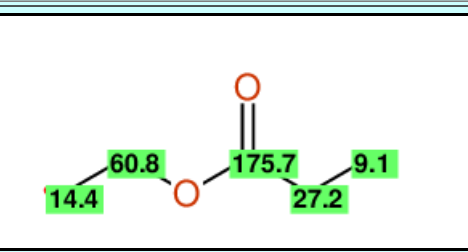




Deviation = 0.87 ppm  
 Similarity = 100 %  
 $C_5H_9O_2$   
 MWT = 101.06  
 Search Web for this structure:  
[IRGLFRDZYNBBCO](#)

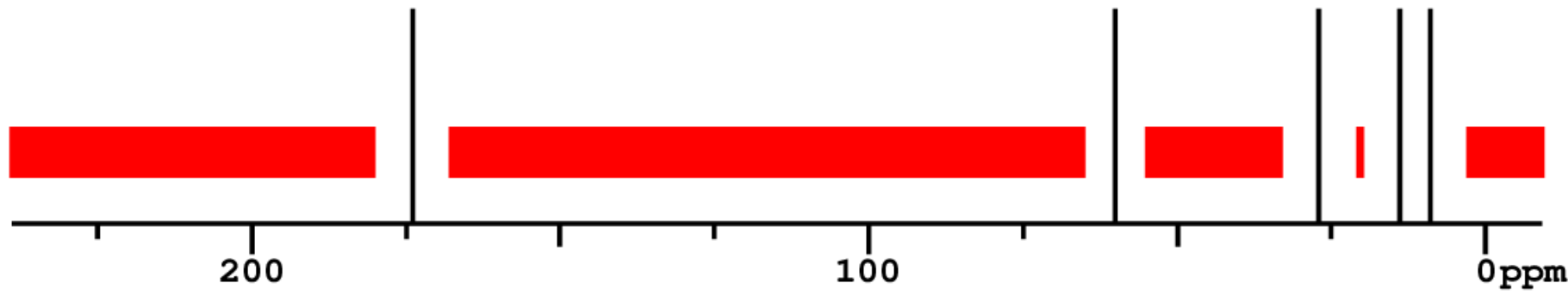
Predicted Chemical Shiftvalues

Matching Map



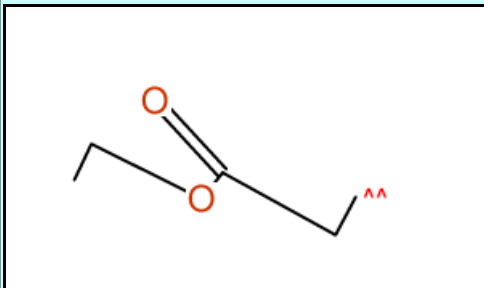
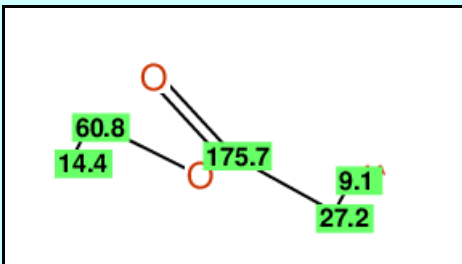
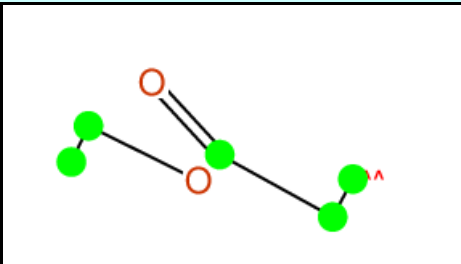
Experimental shift values

No line in reference: 



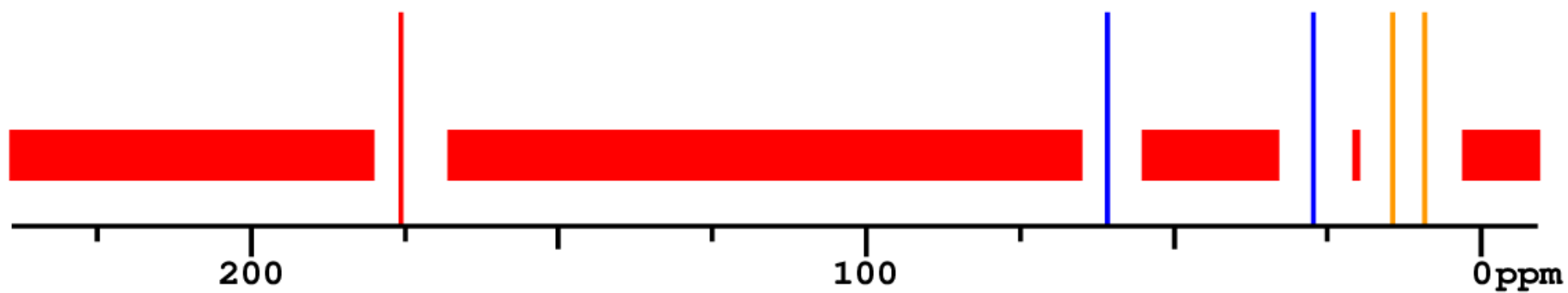
[Back to Complete Result](#)

### Structure Proposal #6

Structure	Similarity Measure
	<p>Deviation = 0.87 ppm Similarity = 100 %</p> <p><math>C_5H_8O_2</math></p> <p>MWT = 100.06</p> <p>Search Web for this structure: <a href="#">BYLOWVUCDFUYIQ</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

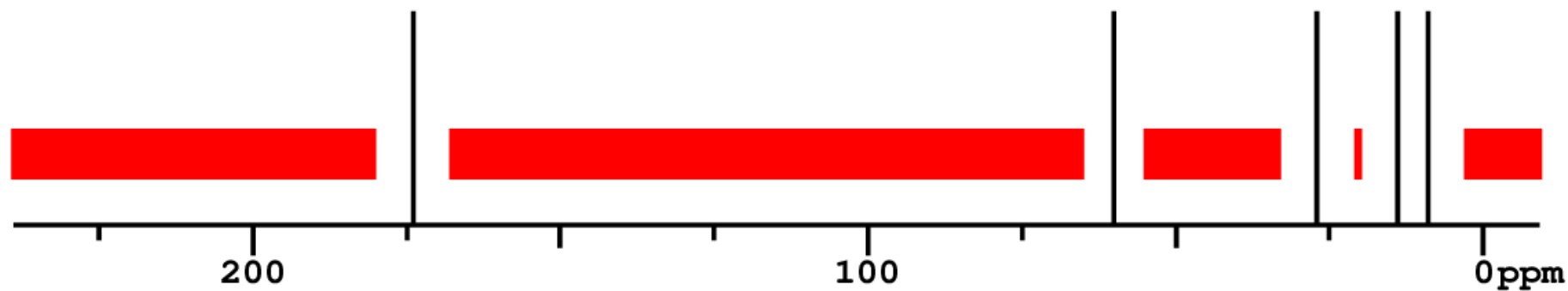
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

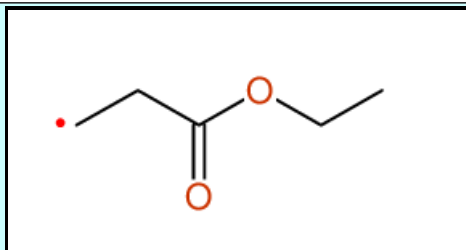
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[Back to Complete Result](#)

### Structure Proposal #7

Structure	Similarity Measure



Deviation = 0.87 ppm  
Similarity = 100 %

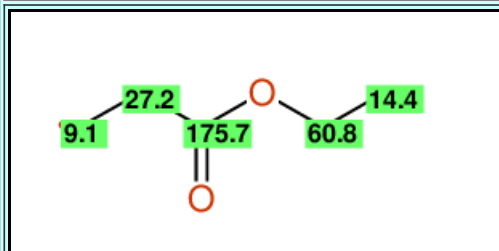
$C_5H_9O_2$

MWT = 101.06

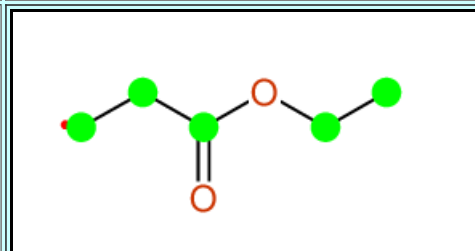
Search Web for this structure:

[SOKCNILPAQLIRC](#)

Predicted Chemical Shiftvalues

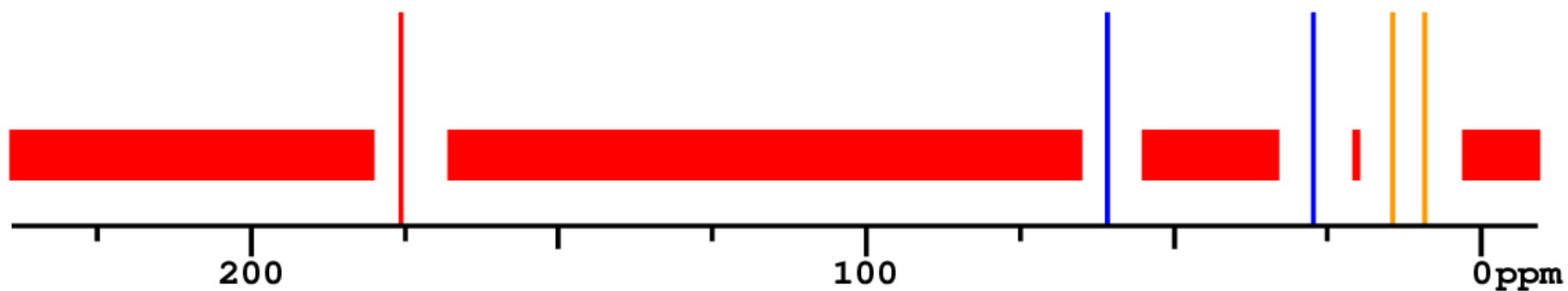


Matching Map



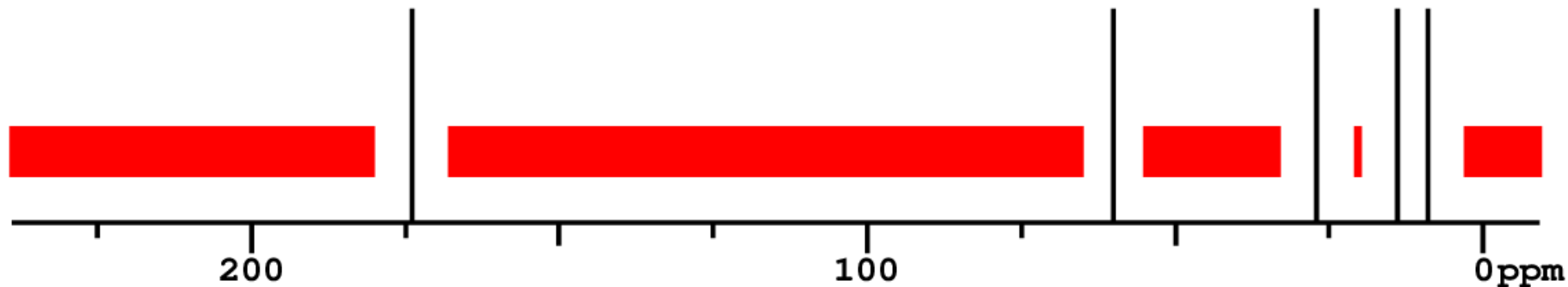
Predicted shift values

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



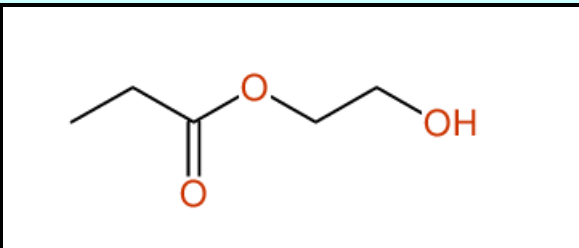
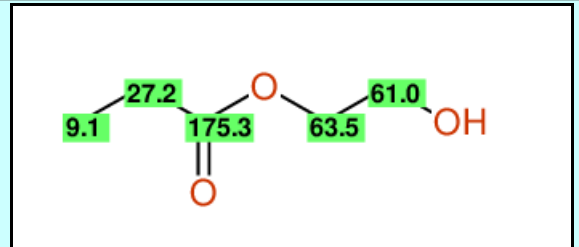
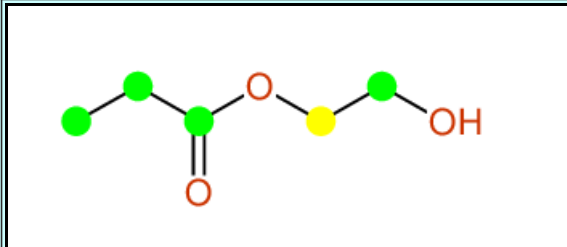
Experimental shift values

No line in reference: 



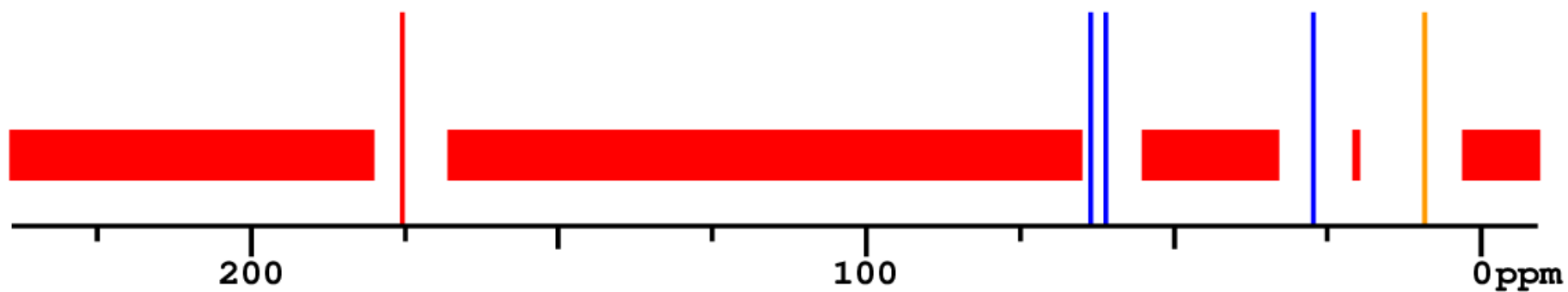
[Back to Complete Result](#)

### Structure Proposal #8

Structure	Similarity Measure
 <chem>CCOC</chem>	Deviation = 2.02 ppm Similarity = 90 %  C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>  MWT = 118.06  Search Web for this structure: <a href="#">SFAMKDPMPDEXGH</a>
Predicted Chemical Shiftvalues	Matching Map
 9.1 27.2 175.3 63.5 61.0	

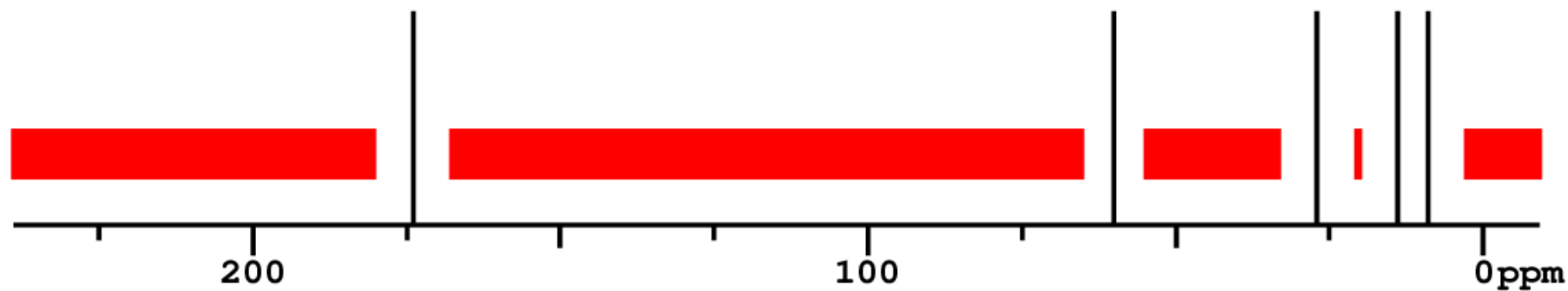
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

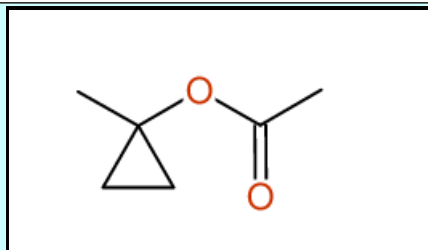
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[Back to Complete Result](#)

### Structure Proposal #9

Structure	Similarity Measure



Deviation = 2.45 ppm

Similarity = 92 %

$C_6H_{10}O_2$

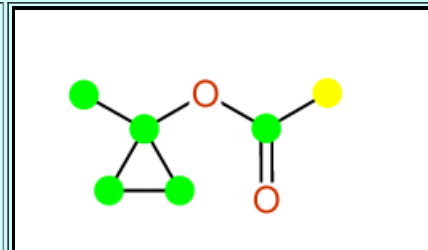
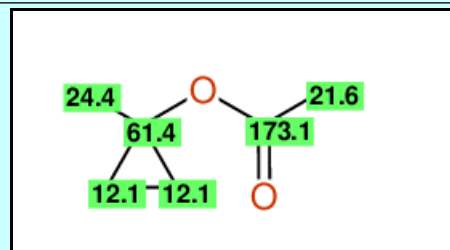
MWT = 114.07

Search Web for this structure:

[MJRMRENRBUEGGM](#)

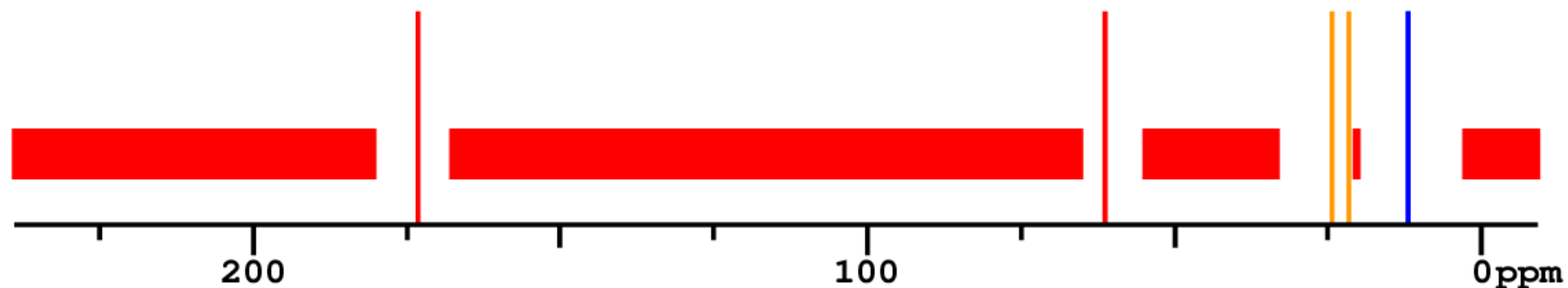
Predicted Chemical Shiftvalues

Matching Map



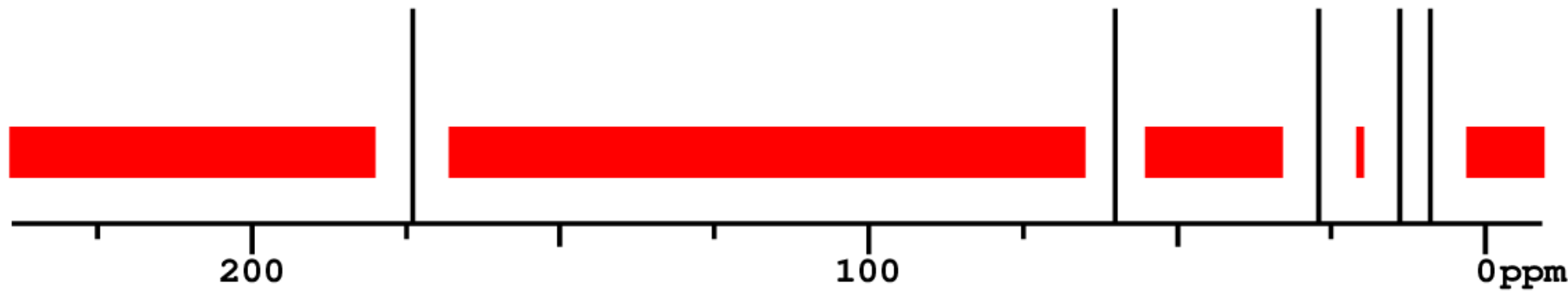
Predicted shift values

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



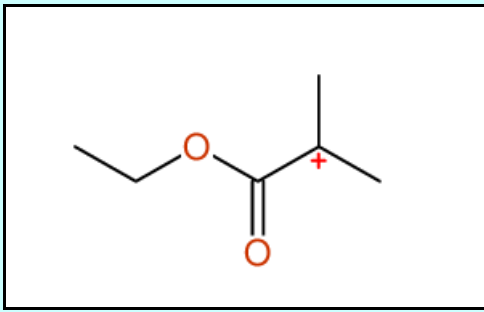
Experimental shift values

No line in reference: 

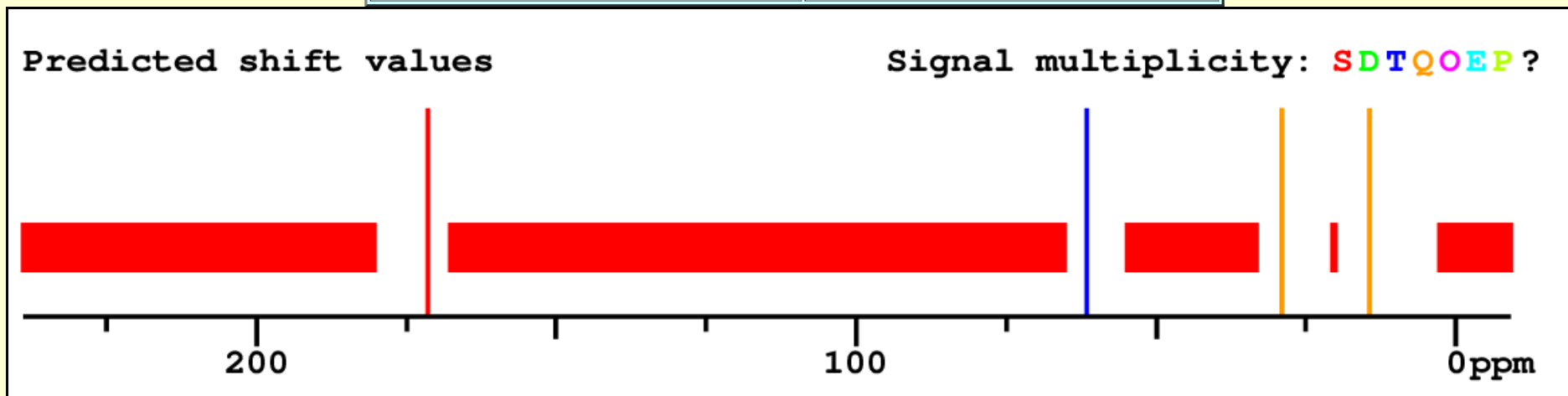
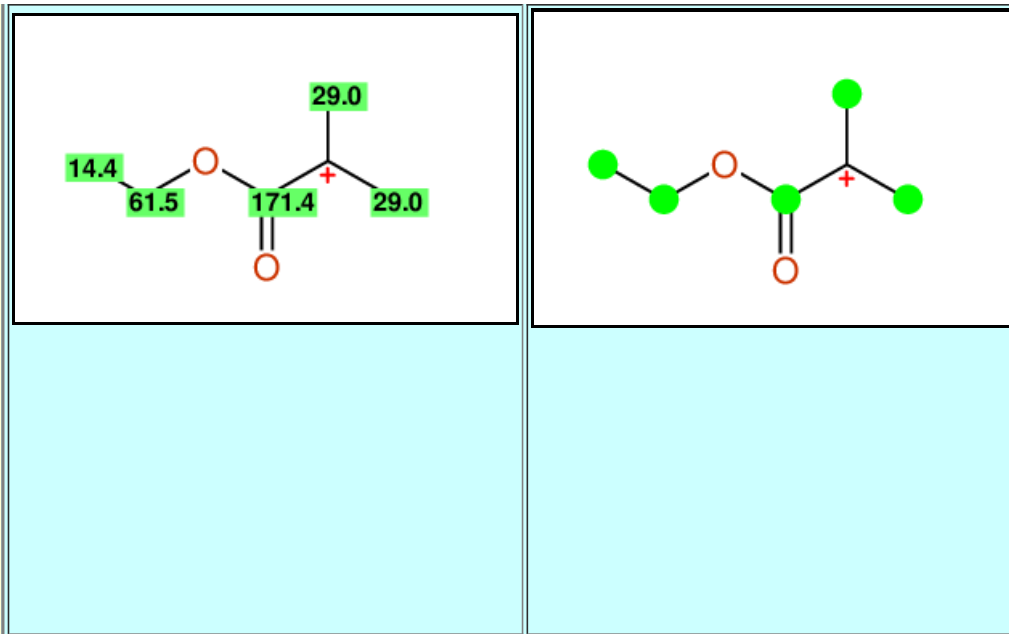


[Back to Complete Result](#)

### Structure Proposal #10

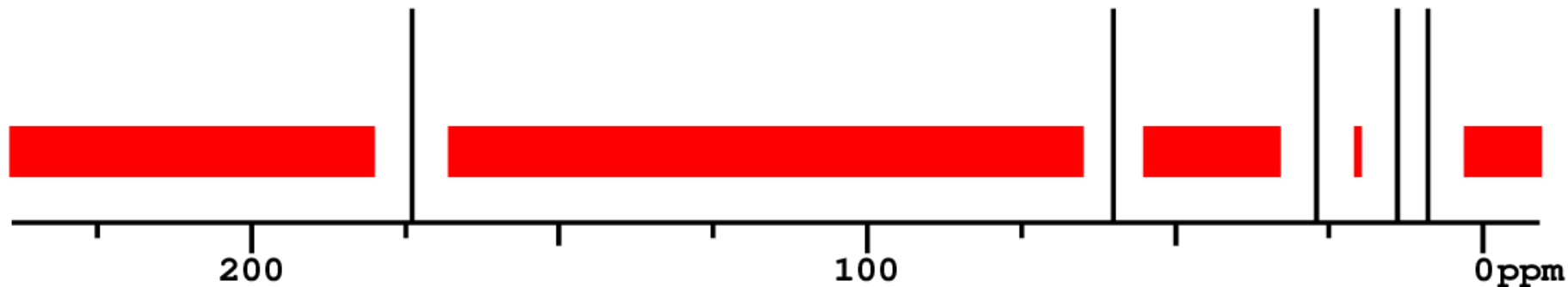
Structure	Similarity Measure
	Deviation = 2.93 ppm Similarity = 100 %  $C_6H_{11}O_2$  MWT = 115.07  Search Web for this structure:  <a href="#">BNJCQKCNZHKCSE</a>
Predicted Chemical Shiftvalues	Matching Map





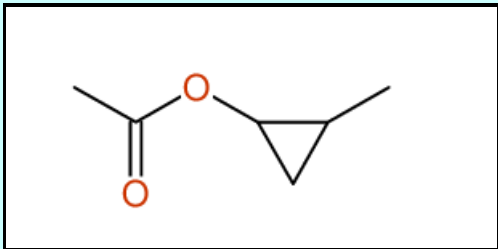
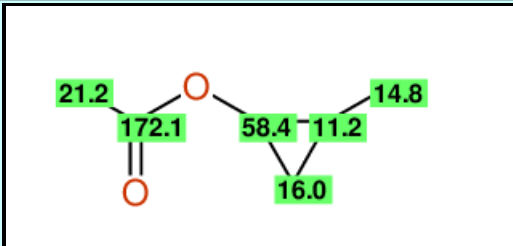
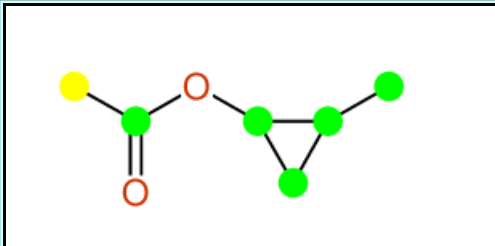
Experimental shift values

No line in reference: 



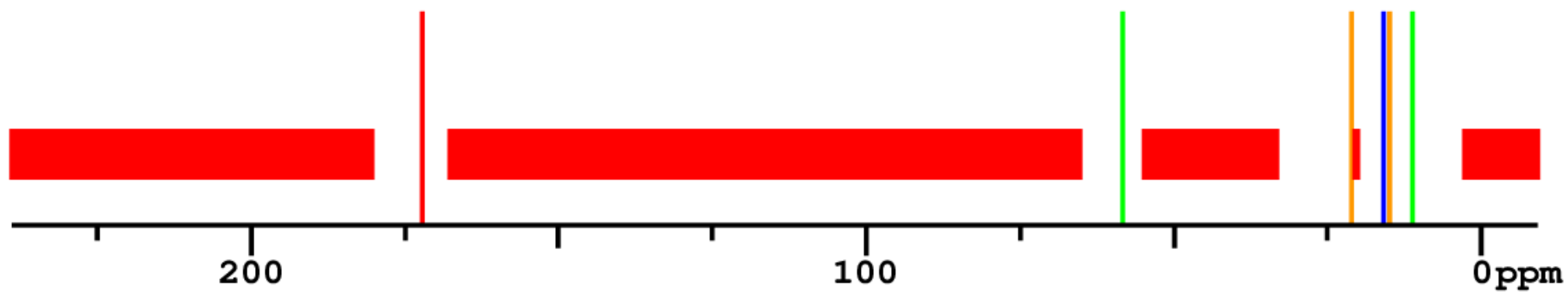
[Back to Complete Result](#)

### Structure Proposal #11

Structure	Similarity Measure
	<p>Deviation = 2.95 ppm Similarity = 92 %</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.07</p> <p>Search Web for this structure: <a href="#">OTXJUSAVQLCSFT</a></p>
Predicted Chemical Shiftvalues	Matching Map
	

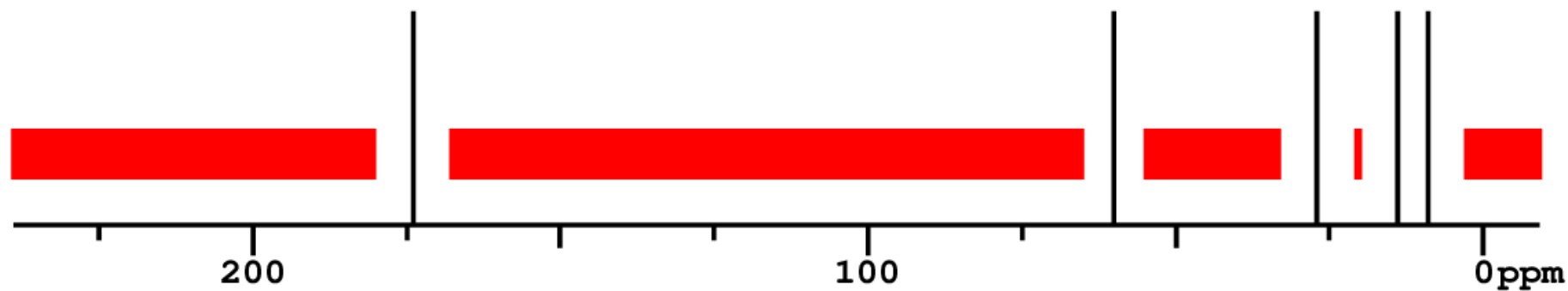
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

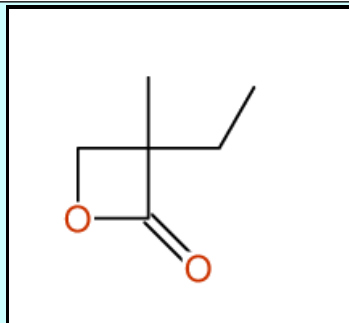
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[Back to Complete Result](#)

### Structure Proposal #12

Structure	Similarity Measure



Deviation = 4.17 ppm  
Similarity = 83 %  
(Different pattern)

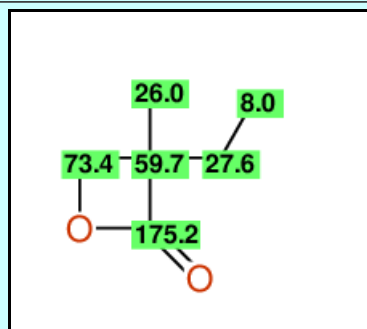


MWT = 114.07

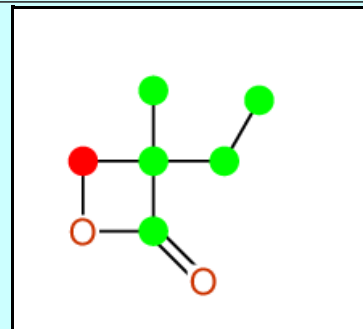
Search Web for this structure:

[UFTRVHTYHBMWOF](#)

Predicted Chemical Shiftvalues

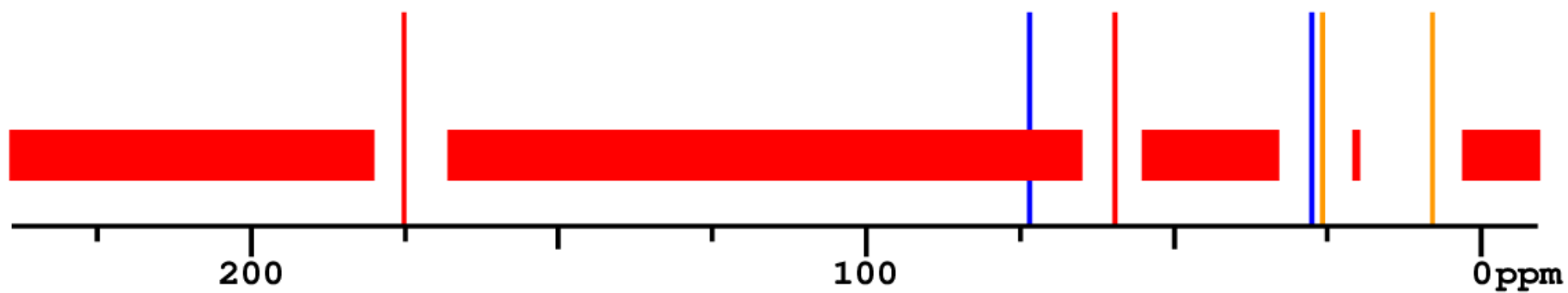


Matching Map



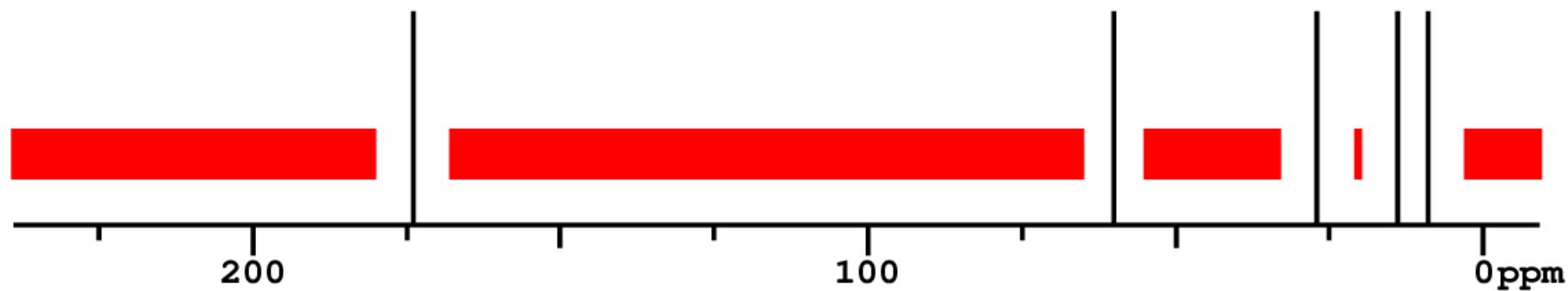
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

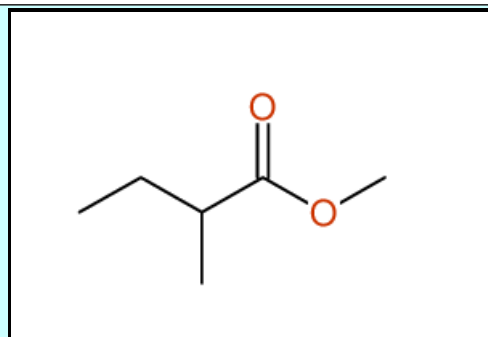
No line in reference: [red bar]



[Back to Complete Result](#)

### Structure Proposal #13

Structure	Similarity Measure



Deviation = 5.25 ppm  
Similarity = 67 %  
(Different pattern)

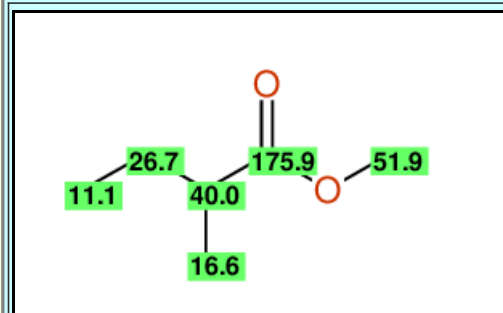


MWT = 114.07

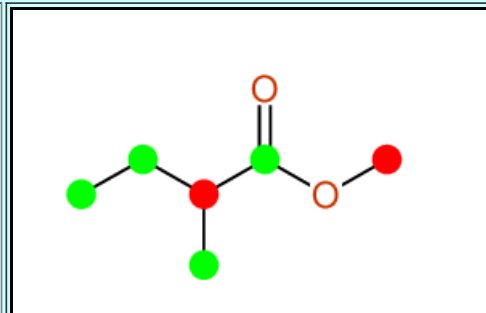
Search Web for this structure:

[YMRCZGBILKTSC](#)

### Predicted Chemical Shiftvalues

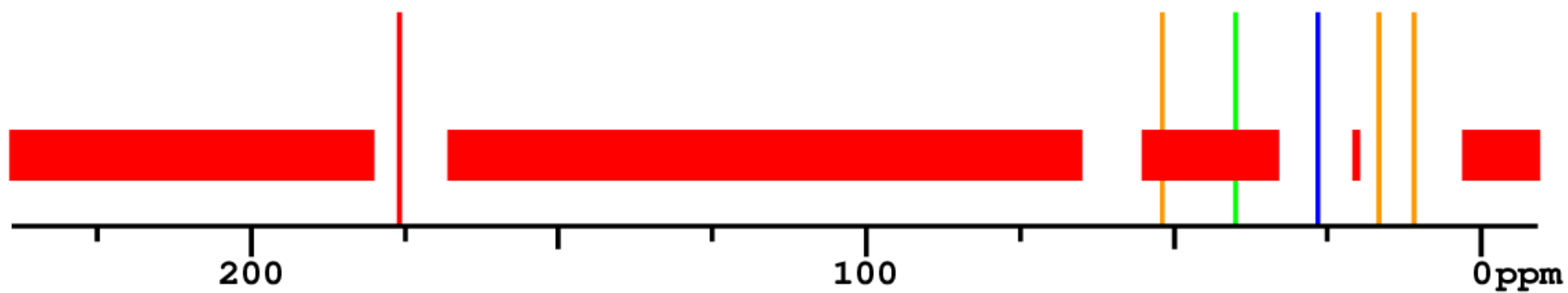


### Matching Map



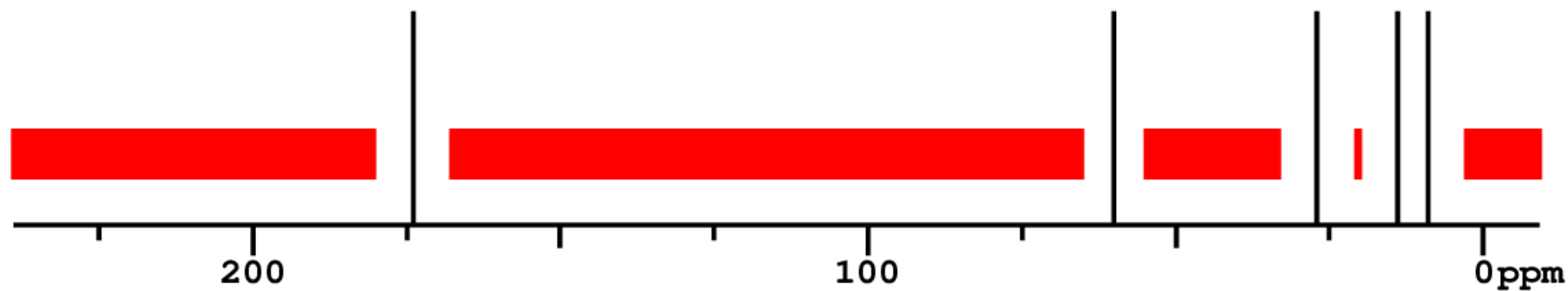
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

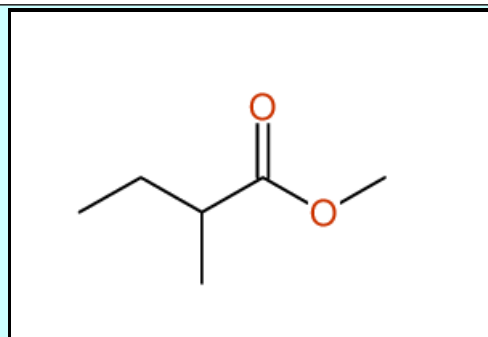
No line in reference:           



[Back to Complete Result](#)

### Structure Proposal #14

Structure	Similarity Measure



Deviation = 5.25 ppm  
Similarity = 67 %  
(Different pattern)

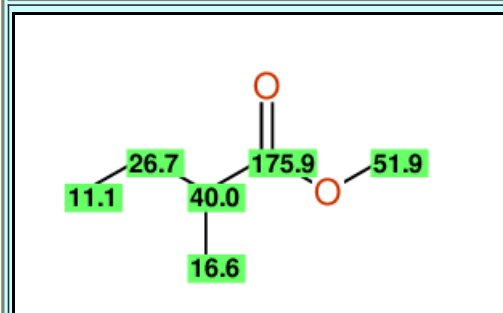


MWT = 114.07

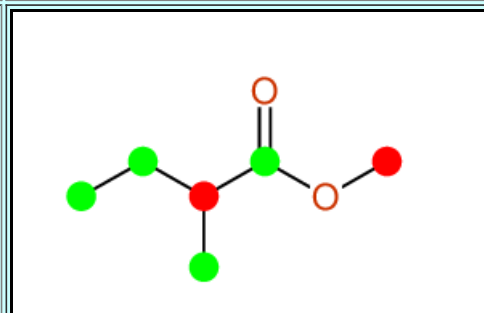
Search Web for this structure:

[OYGDMLWQJBKWLN](#)

#### Predicted Chemical Shiftvalues



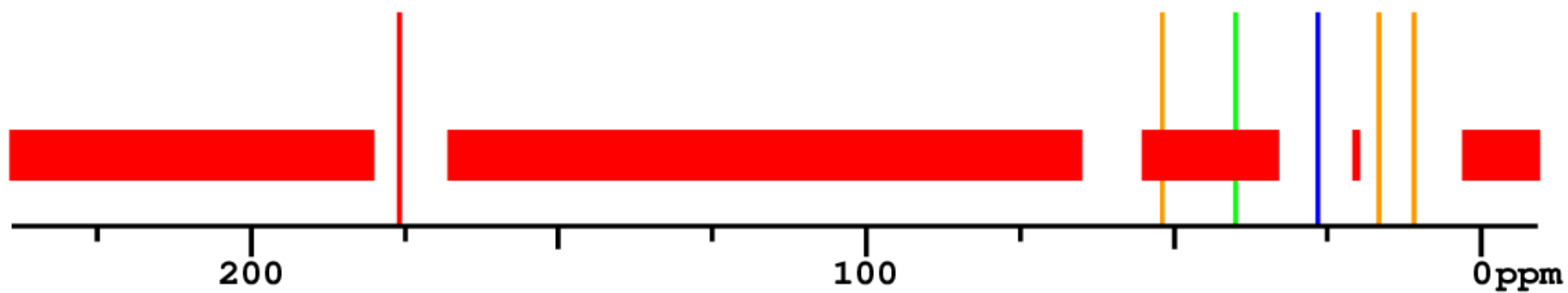
#### Matching Map





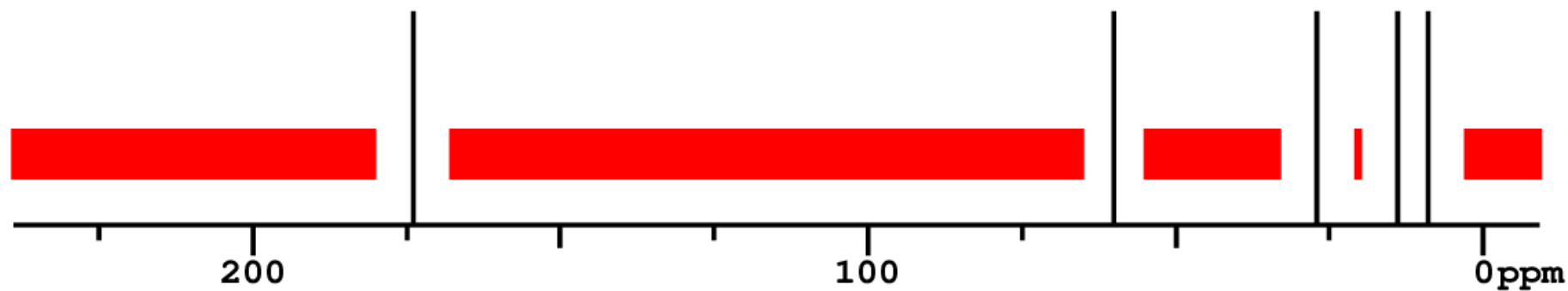
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

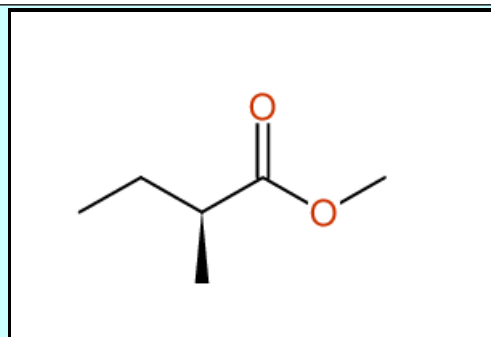
No line in reference:           



[Back to Complete Result](#)

### Structure Proposal #15

Structure	Similarity Measure



Deviation = 5.25 ppm  
 Similarity = 67 %  
 (Different pattern)



MWT = 116.07

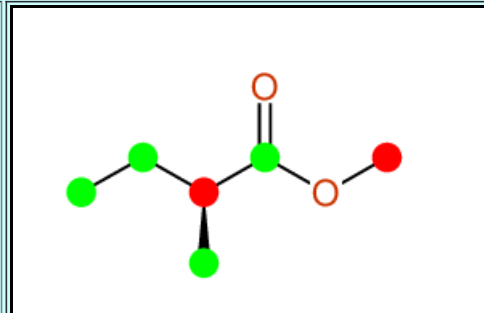
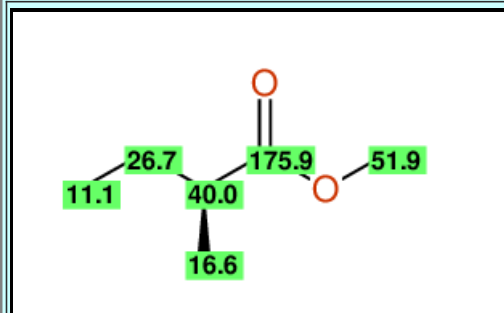
Search Web for this structure:

[OCWLYWIFNDCWRZ](#)

[Availability](#)

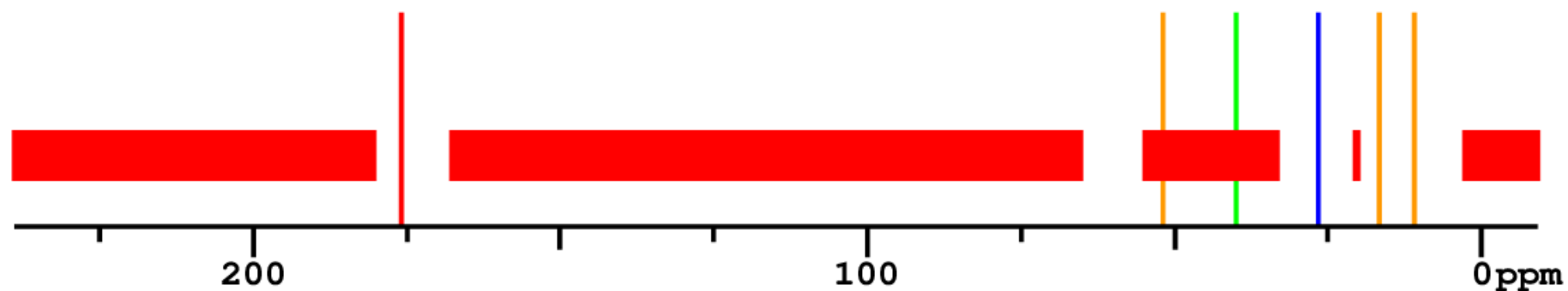
Predicted Chemical Shiftvalues

Matching Map



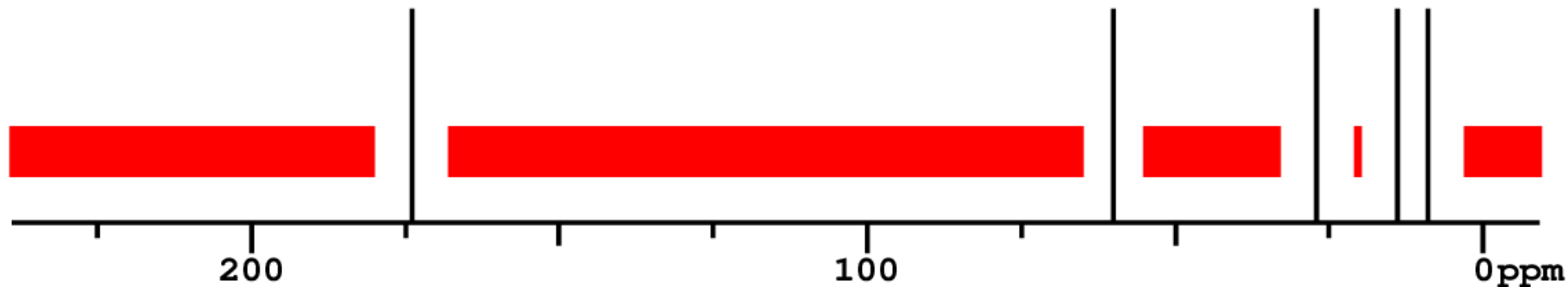
Predicted shift values

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



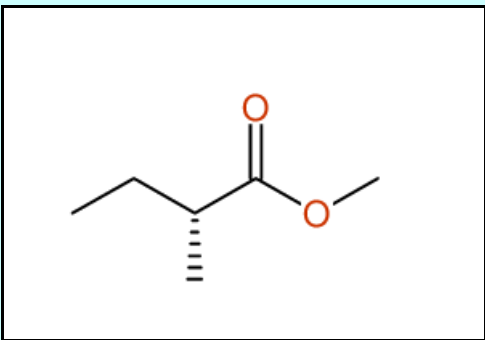
Experimental shift values

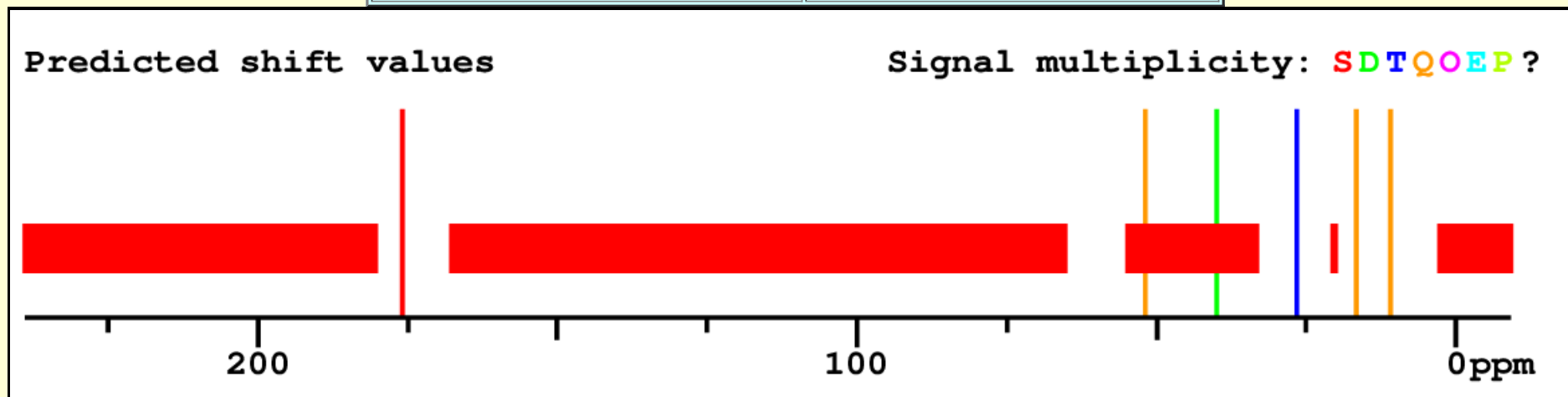
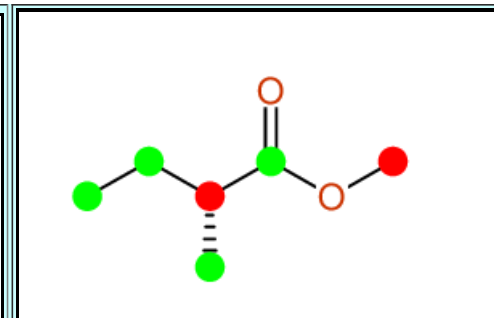
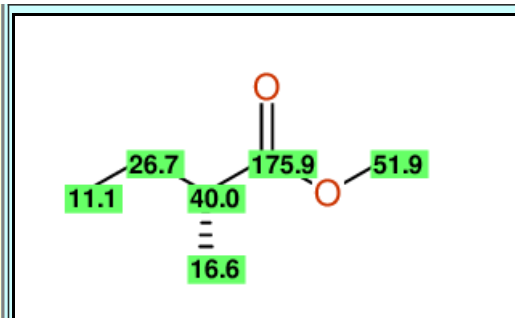
No line in reference: 



[Back to Complete Result](#)

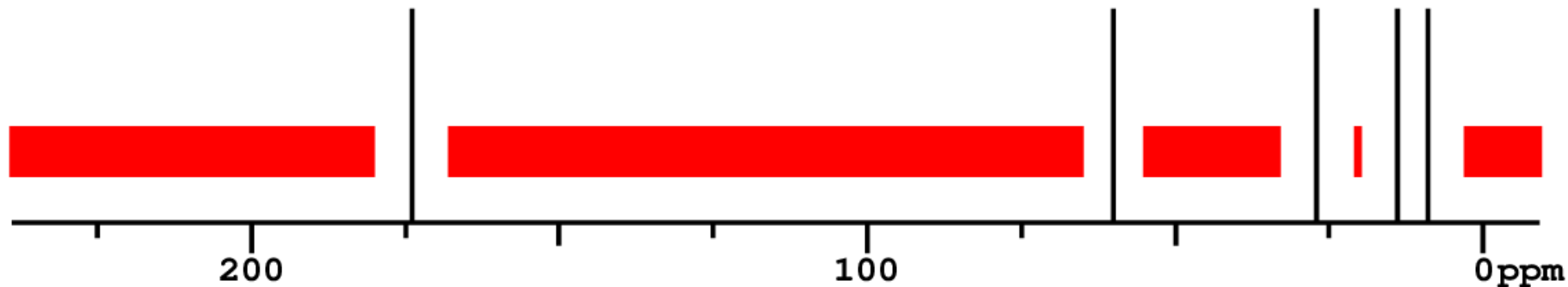
### Structure Proposal #16

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.07</p> <p>Search Web for this structure: <a href="#">OCWLYWIFENDCWRZ</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



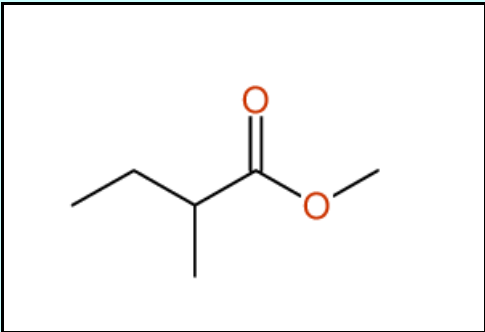
Experimental shift values

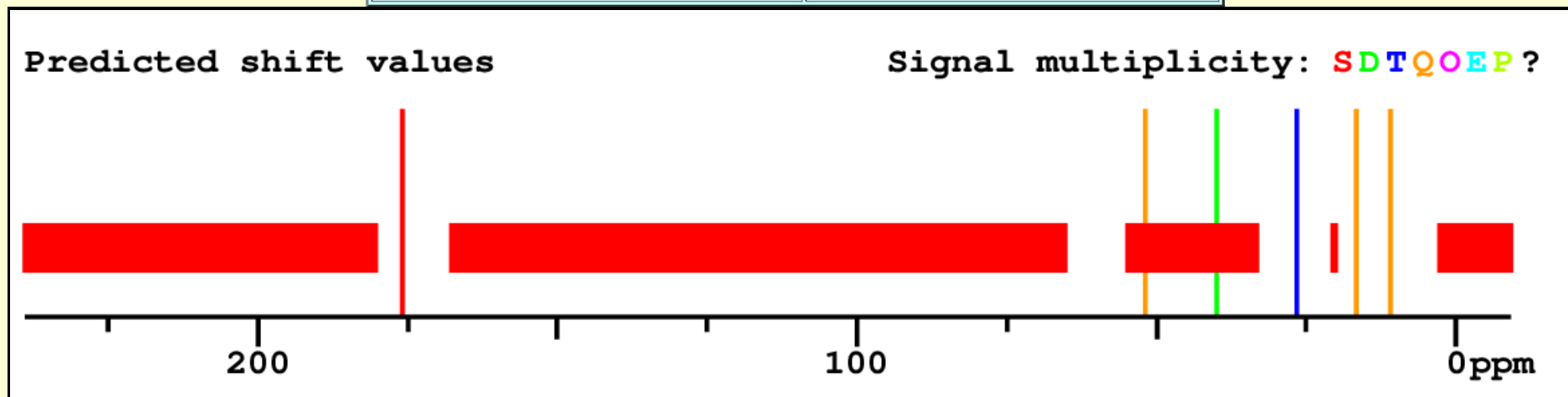
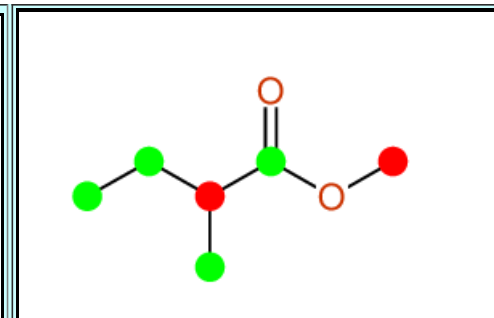
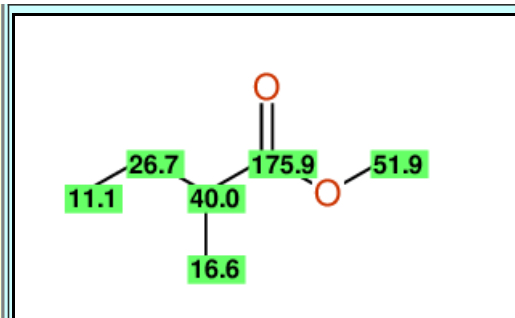
No line in reference: 




[Back to Complete Result](#)

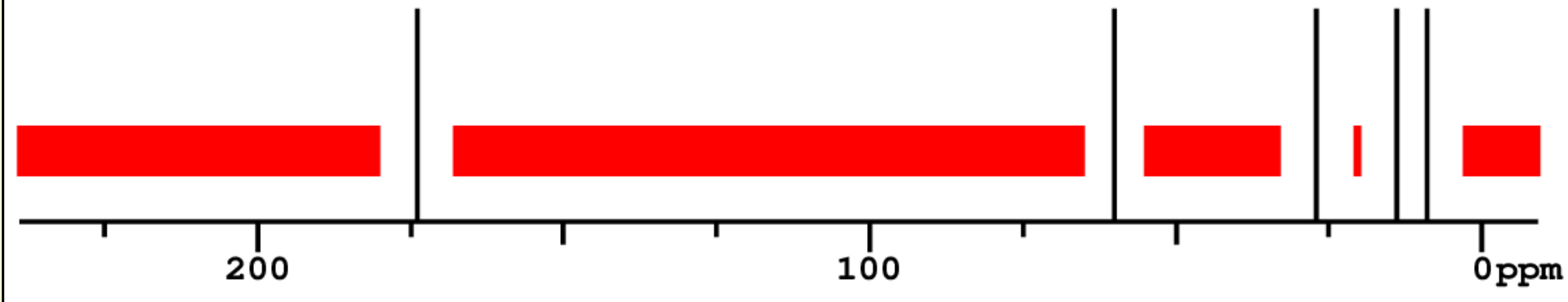
### Structure Proposal #17

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{12}O_2</math></p> <p>MWT = 116.07</p> <p>Search Web for this structure: <a href="#">OCWLYWIFENDCWRZ</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



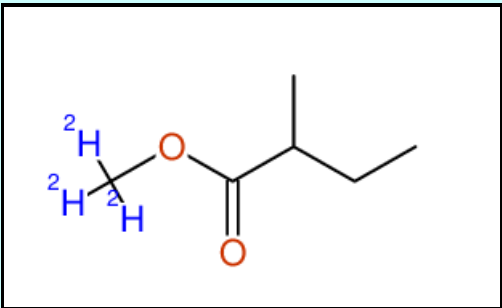
Experimental shift values

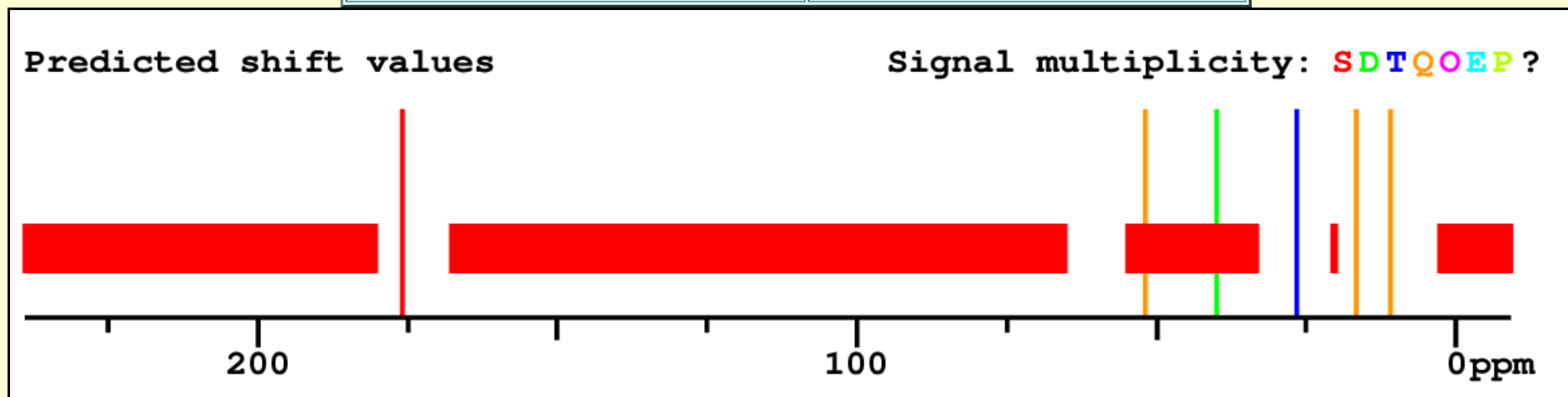
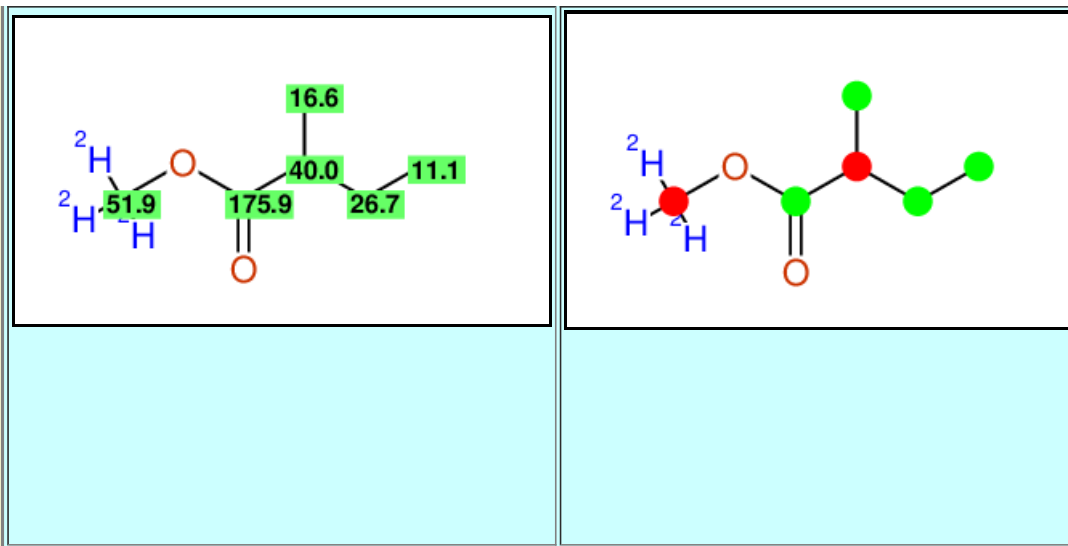
No line in reference: 



[Back to Complete Result](#)

### Structure Proposal #18

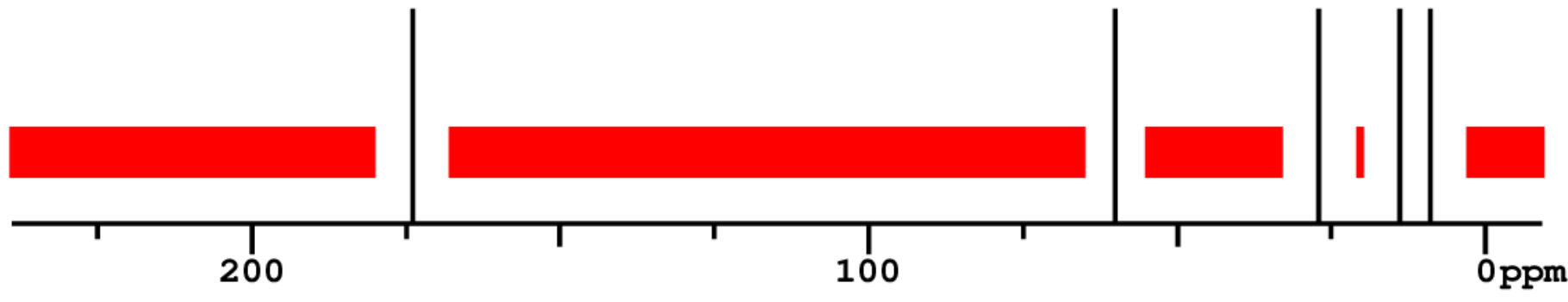
Structure	Similarity Measure
	<p>Deviation = 5.25 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{12}O_2</math></p> <p>MWT = 119.07</p> <p>Search Web for this structure: <a href="#">OCWLYWIFNDCWRZ</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map





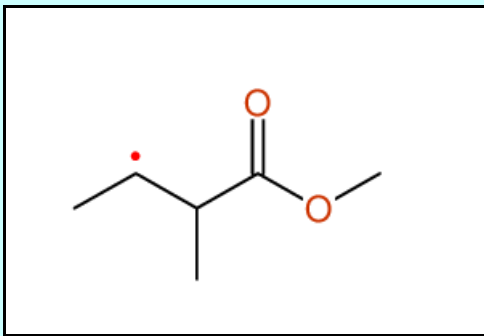
Experimental shift values

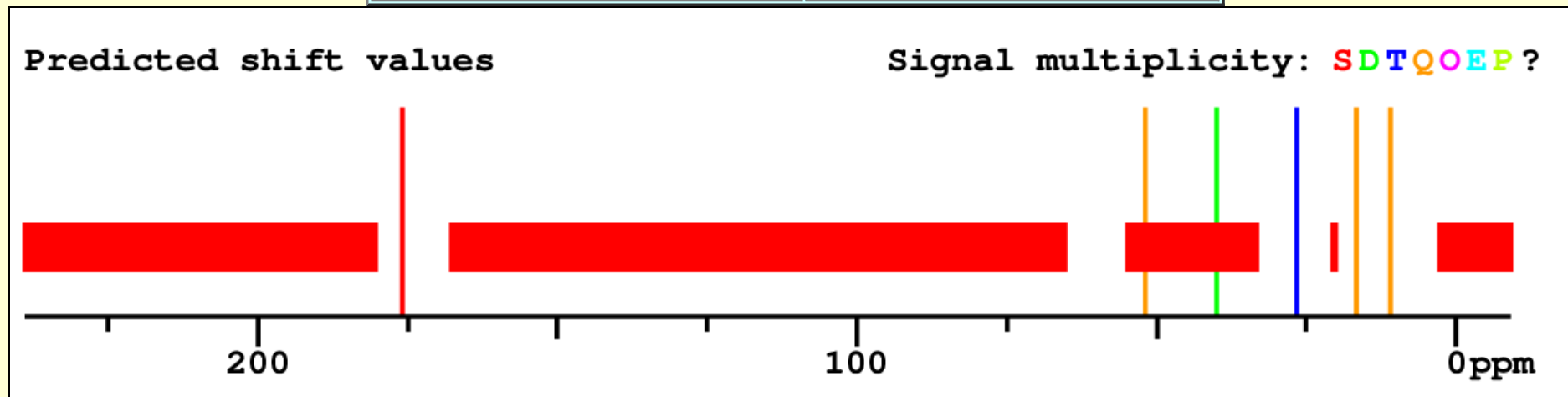
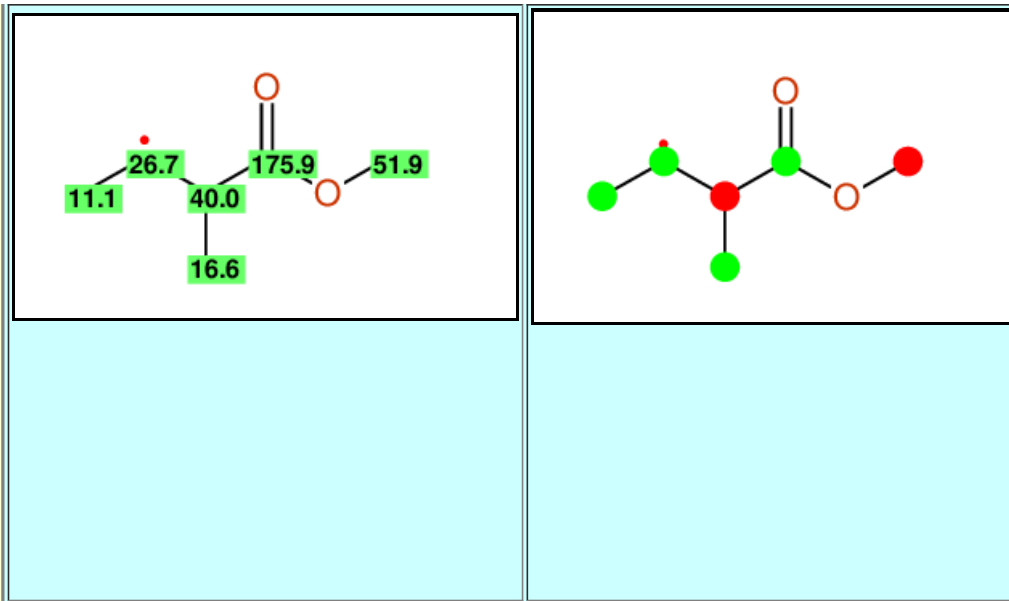
No line in reference: 



[Back to Complete Result](#)

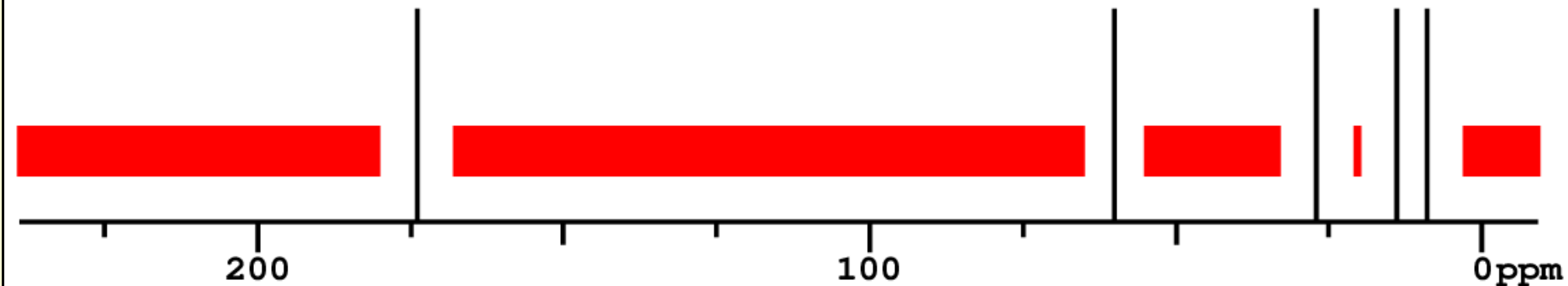
### Structure Proposal #19

Structure	Similarity Measure
	<p>Deviation = 5.25 ppm Similarity = 67 % (Different pattern)</p> <p><math>C_6H_{11}O_2</math></p> <p>MWT = 115.07</p> <p>Search Web for this structure: <a href="#">WKWGMFVUDZAZEV</a></p>
Predicted Chemical Shiftvalues	Matching Map



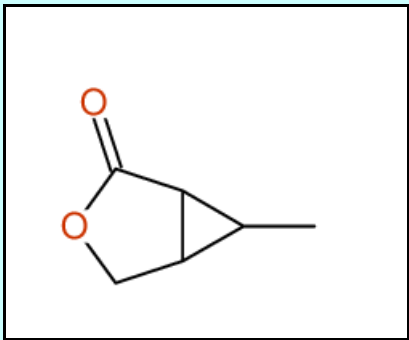
Experimental shift values

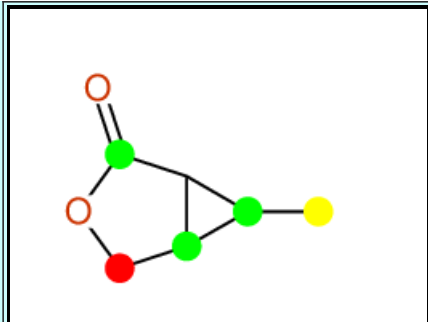
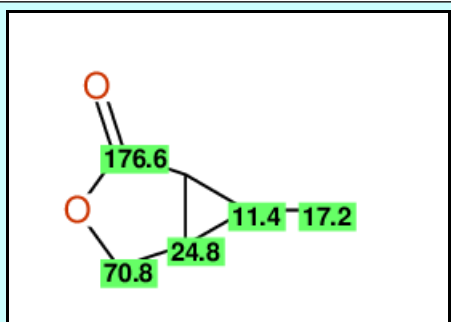
No line in reference: 



[Back to Complete Result](#)

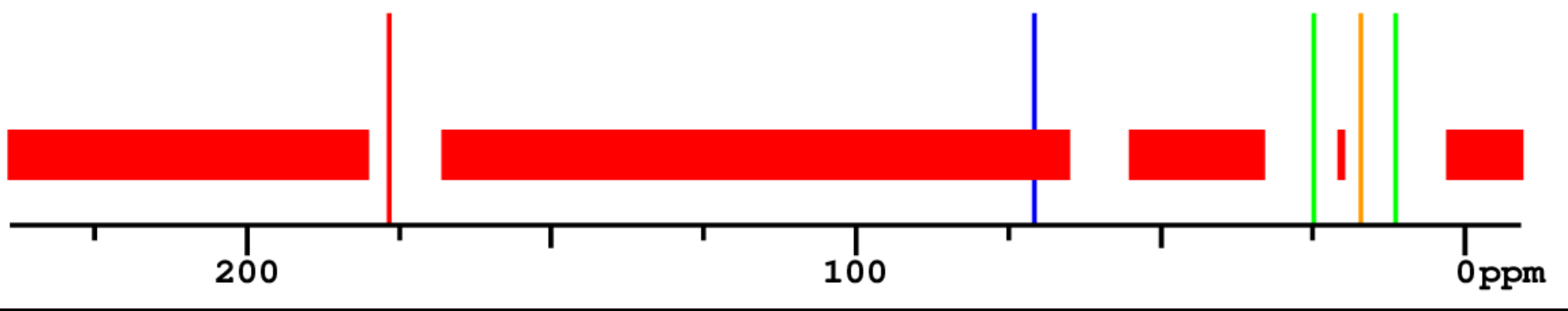
### Structure Proposal #20

Structure	Similarity Measure
	<p>Deviation = 5.38 ppm Similarity = 70 % (Different pattern)</p> <p><math>C_6H_8O_2</math></p> <p>MWT = 112.07</p> <p>Search Web for this structure: <a href="#">ODZSNSOKRZBPDY</a></p>
Predicted Chemical Shiftvalues	Matching Map



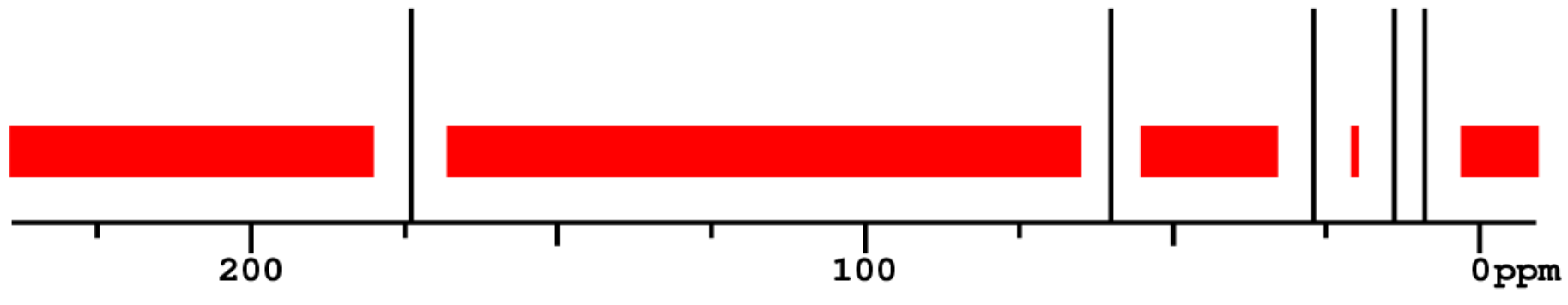
Predicted shift values

Signal multiplicity: S D T Q O E P ?



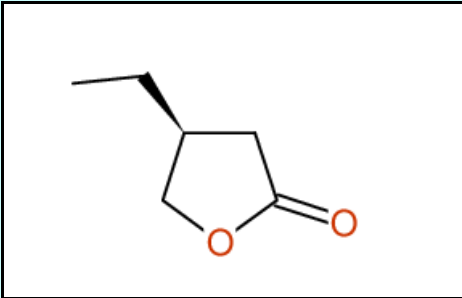
Experimental shift values

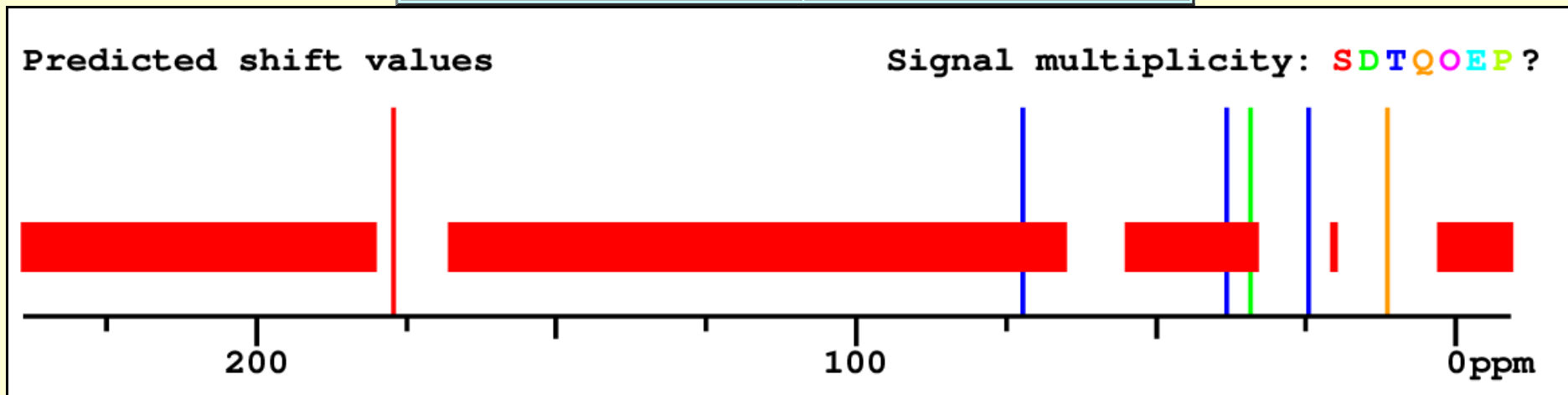
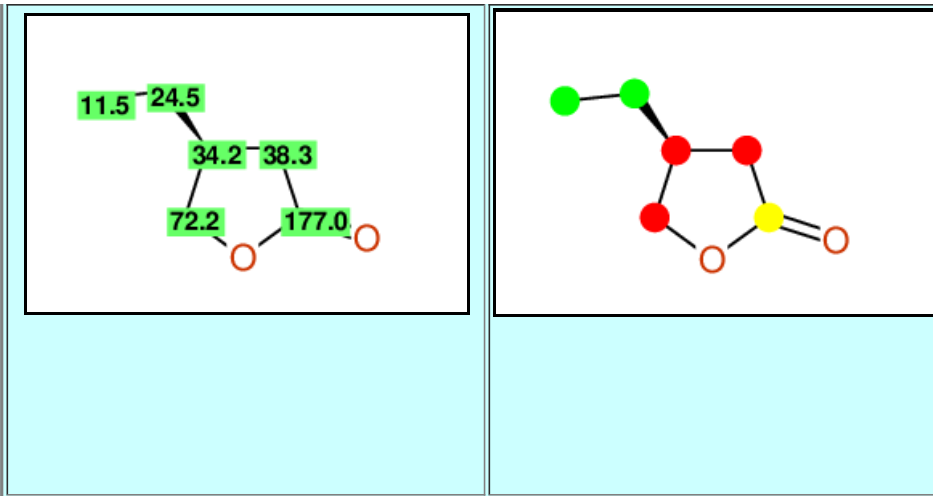
No line in reference: 



[Back to Complete Result](#)

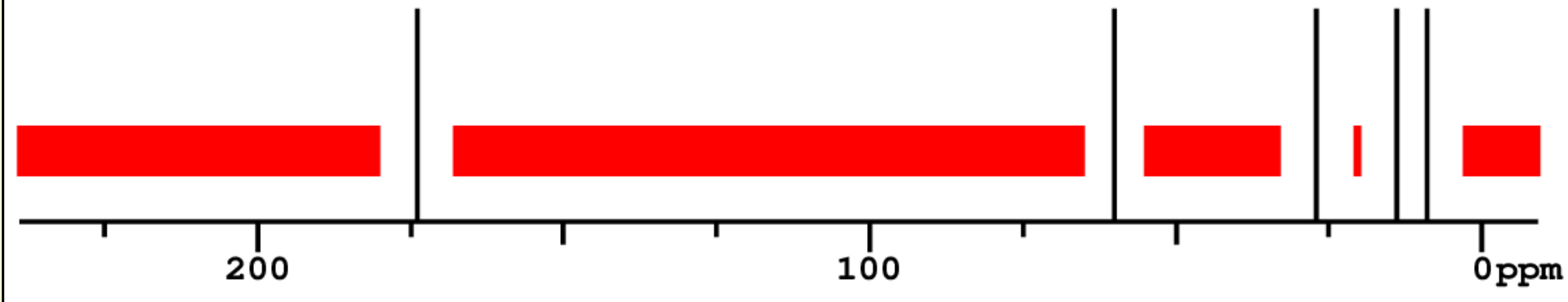
### Structure Proposal #21

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



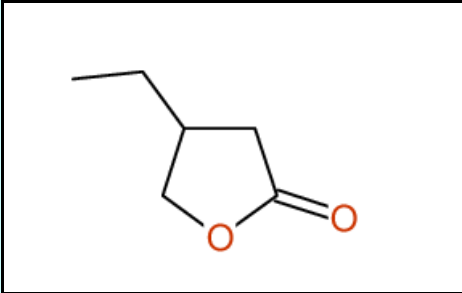
Experimental shift values

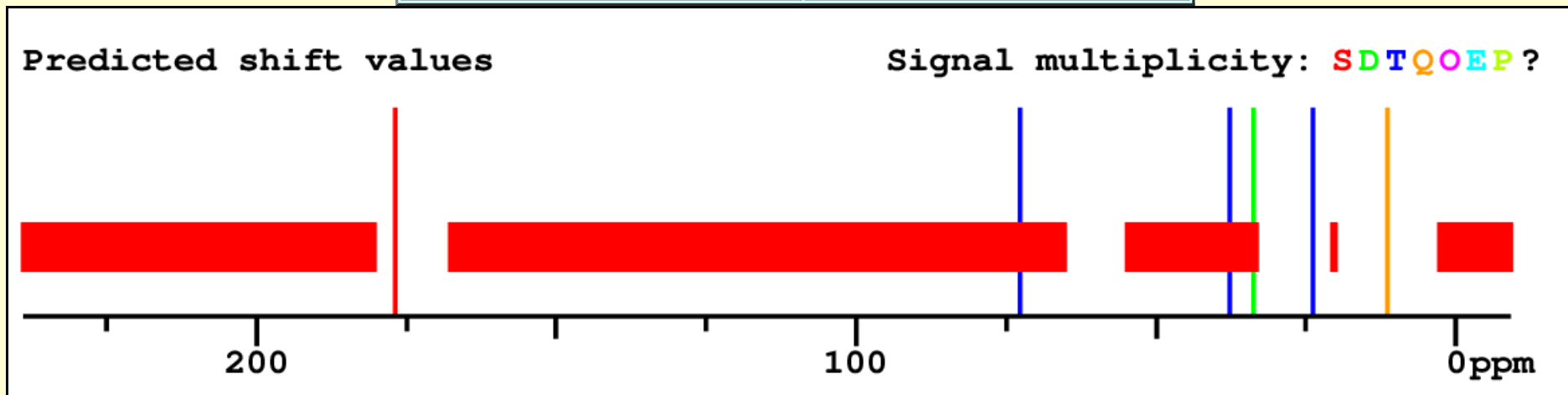
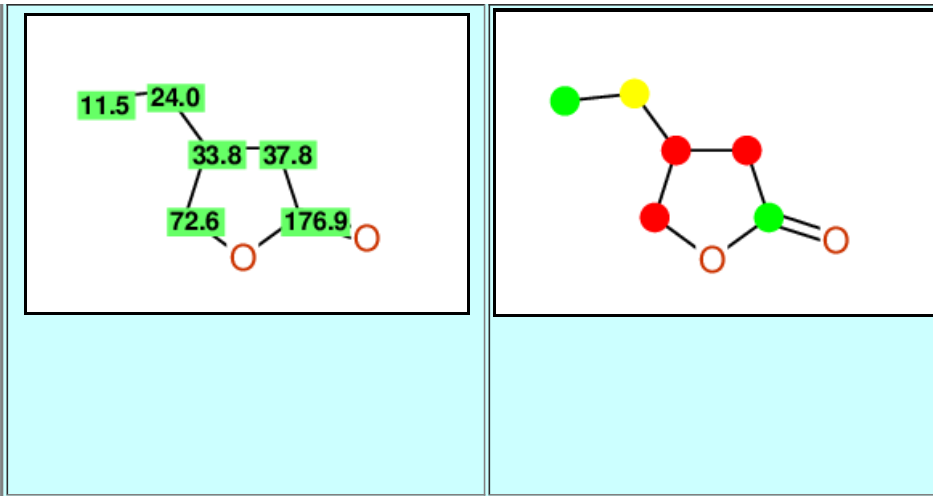
No line in reference: 



[Back to Complete Result](#)

### Structure Proposal #22

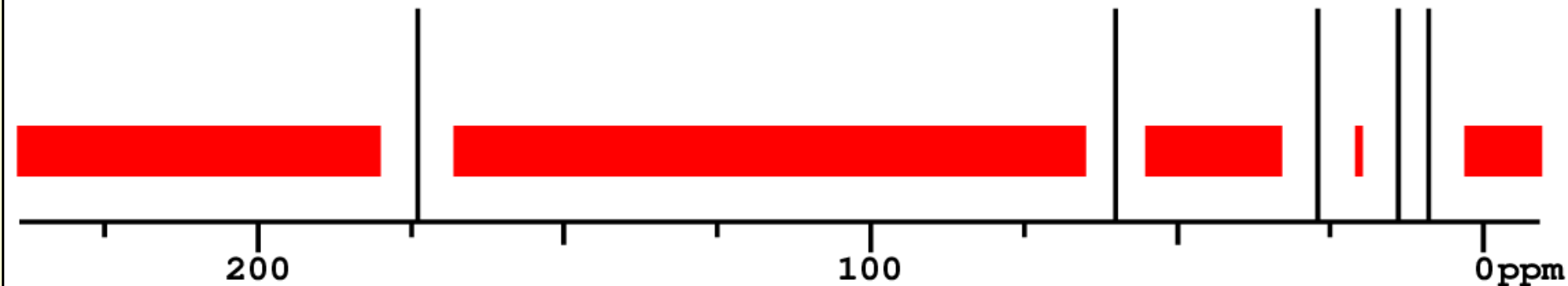
Structure	Similarity Measure
	<p>Deviation = 6.88 ppm Similarity = 42 % (Different pattern)</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.07</p> <p>Search Web for this structure: <a href="#">MDQZVJSUBKPTHG</a></p> <p><a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map





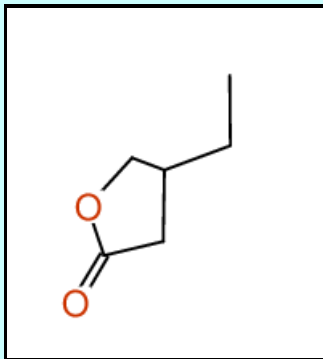
Experimental shift values

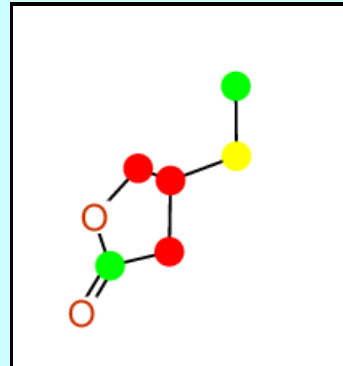
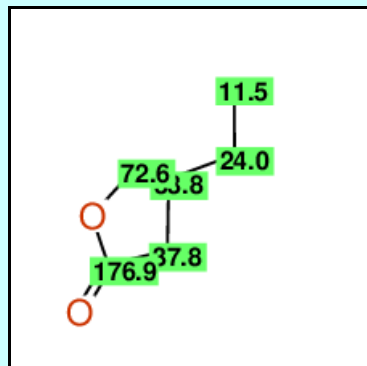
No line in reference: 



[Back to Complete Result](#)

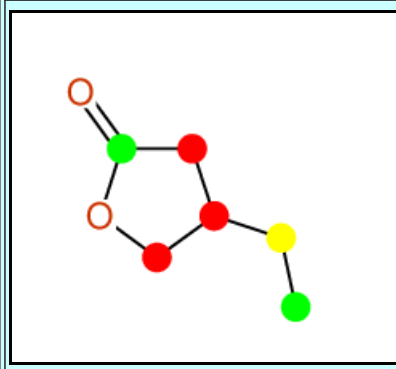
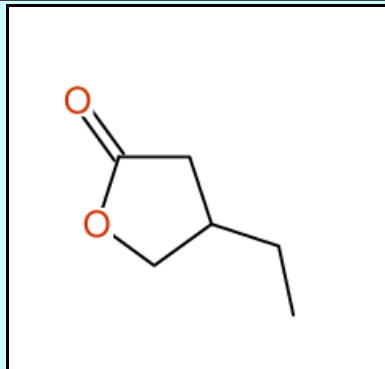
### Structure Proposal #23

Structure	Similarity Measure
	<p>Deviation = 6.88 ppm Similarity = 42 % (Different pattern)</p> <p><math>C_6H_{10}O_2</math></p> <p>MWT = 114.07</p> <p>Search Web for this structure: <a href="#">MDQZVJSUBKPTHG</a> <a href="#">Availability</a></p>
Predicted Chemical Shiftvalues	Matching Map



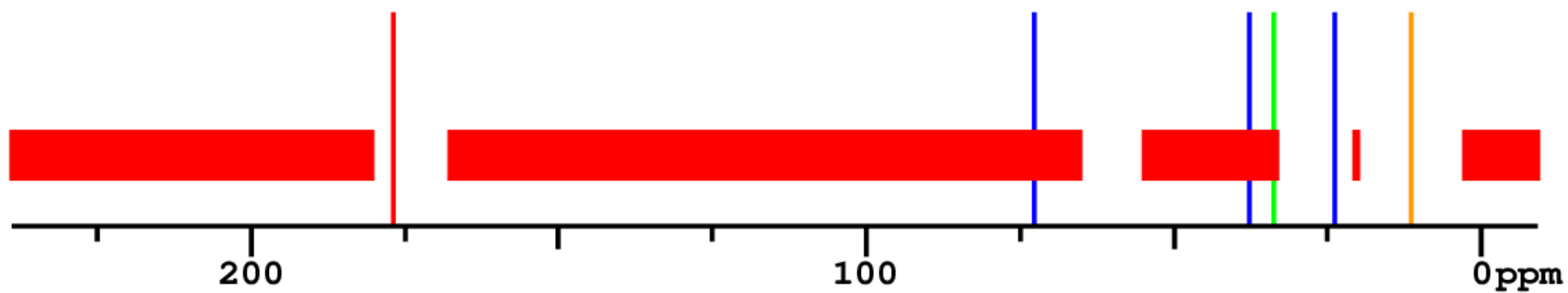
2D Structure Representation

2D Matching Map



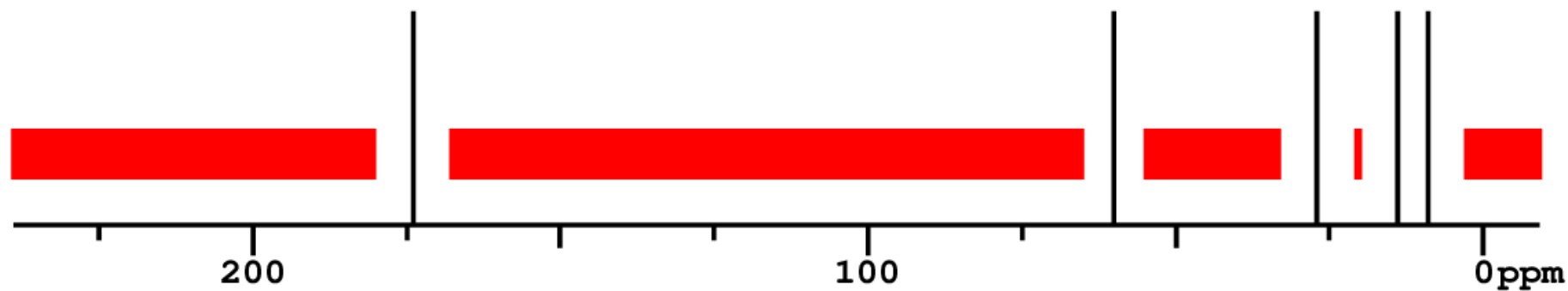
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

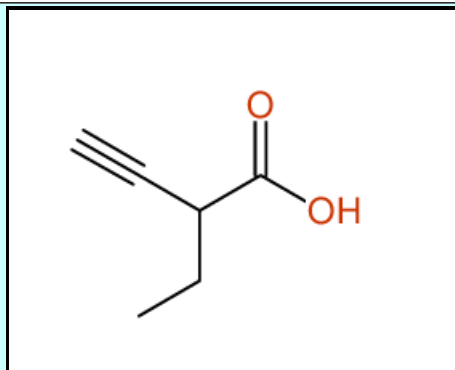
No line in reference: [red bar]



[Back to Complete Result](#)

### Structure Proposal #24

Structure	Similarity Measure



Deviation = 8.49 ppm  
Similarity = 50 %  
(Different pattern)

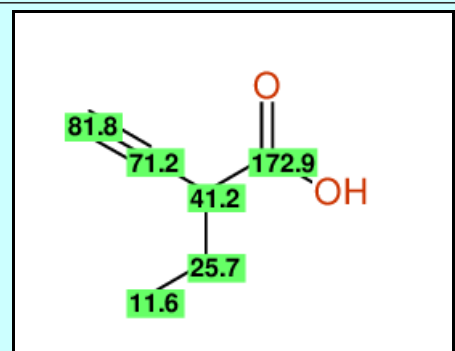


MWT = 112.07

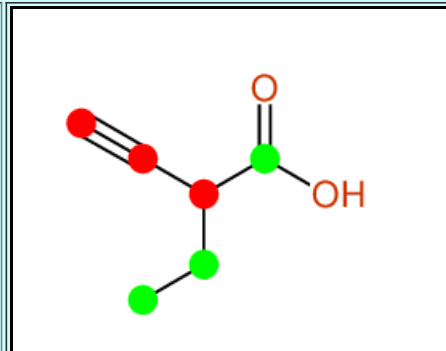
Search Web for this structure:

[YHXLBJJLZTWBAZ](https://www.google.com/search?q=YHXLBJJLZTWBAZ)

Predicted Chemical  
Shiftvalues

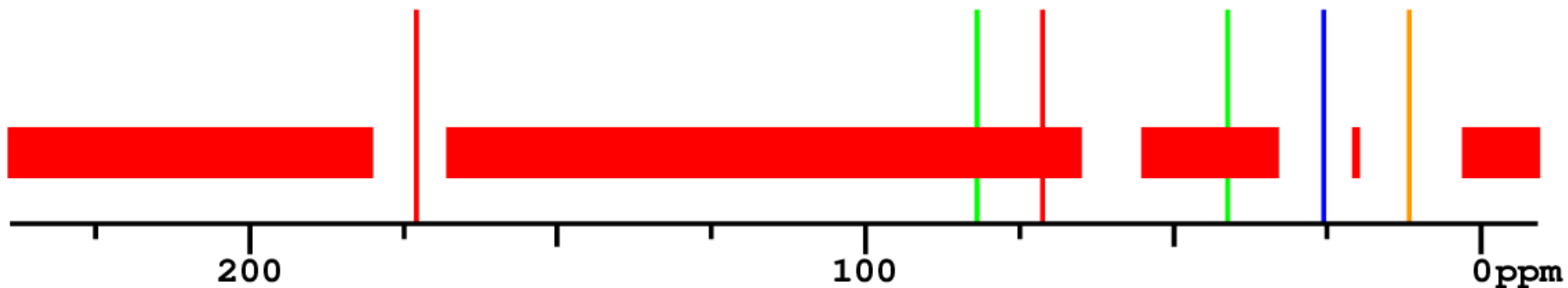


Matching Map



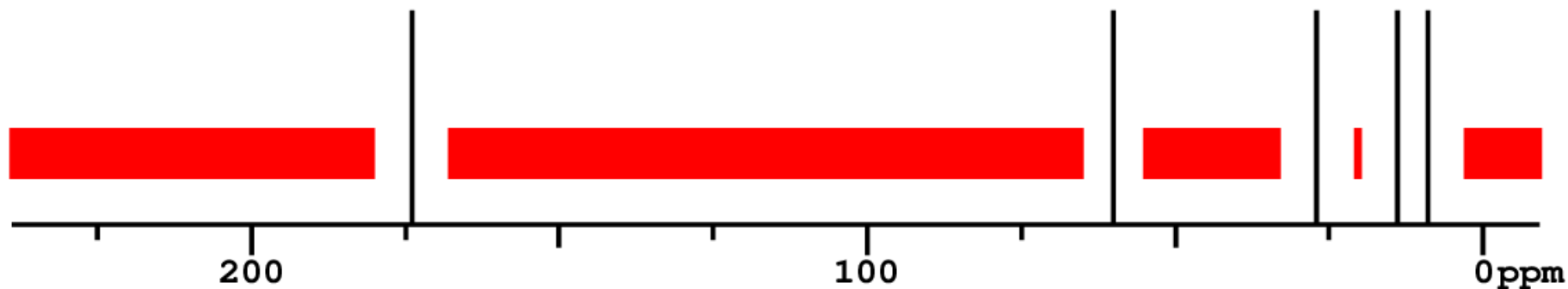
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

No line in reference: [red bar]



[Back to Complete Result](#)

Summary of the 2 most frequently occurring parent ring systems  
within the 11 best-fitting entries

Occurrence:

1 in 11



Occurrence:

1 in 11



Summary of the 4 most frequently occurring parent ring systems  
within the 20 best-fitting entries

Occurrence:

1 in 20



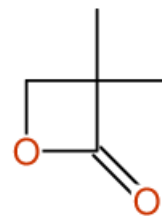
Occurrence:

1 in 20



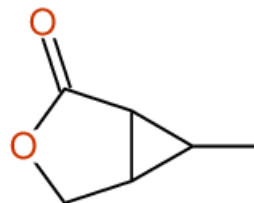
Occurrence:

1 in 20



Occurrence:

1 in 20



## Summary of Processing

Checking existence of data and counting them:

107,426,223 entries in 2.338 seconds

<b>Applying restraints from elemental composition:</b>	<b>7.247 seconds, 3,176,524 entries remain</b>
<b>Applying restraints from number of signals:</b>	<b>2.356 seconds, 222,114 entries remain</b>
<b>Searching 1,956,285,417 chemical shift values line-per-line:</b>	<b>27.290 seconds</b>
<b>Best 2,194 entries selected for analysis:</b>	<b>2.541 seconds</b>
<b>Ranking of 2,194 entries by similarity:</b>	<b>87.067 seconds</b>
<b>Deviation of best match:</b>	<b>0.87 ppm</b>
<b>Creating table and linking 2,194 structures to 475,803 INCHIKEY-pages:</b>	<b>1.012 seconds</b>
<b>Detailed Analysis of 24 structures including graphical representation:</b>	<b>8.141 seconds</b>
<b>Analysis of 20 structures for common parent ring systems:</b>	<b>0.005 seconds</b>
<b>Total CPU-usage:</b>	<b>138.923 seconds</b>
<b>Data transferred from disk:</b>	<b>1,526 MBytes out of 1,695,823 MBytes</b>
<b>Program version:</b>	<b>20200916_2-3D-zip/00</b>
<b>Machine:</b>	<b>I9-9900K / 16x3.60GHz</b>
<p><b>Page written by Wolfgang Robien using CSEARCH-Technology</b>  <b>Page written on 2021:05:19 at 19:09</b>  <b>Page finished on 2021:05:19 at 19:14</b></p> <p><b>Have a nice day !</b></p>	