

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

Description of Request

Please cite this service as:

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

Automatic Resubmit:

Multiplicity omitted

Request submitted via:



Requested by:

test@test123.abc.info

Requested on:

2021:05:19 at 19:09

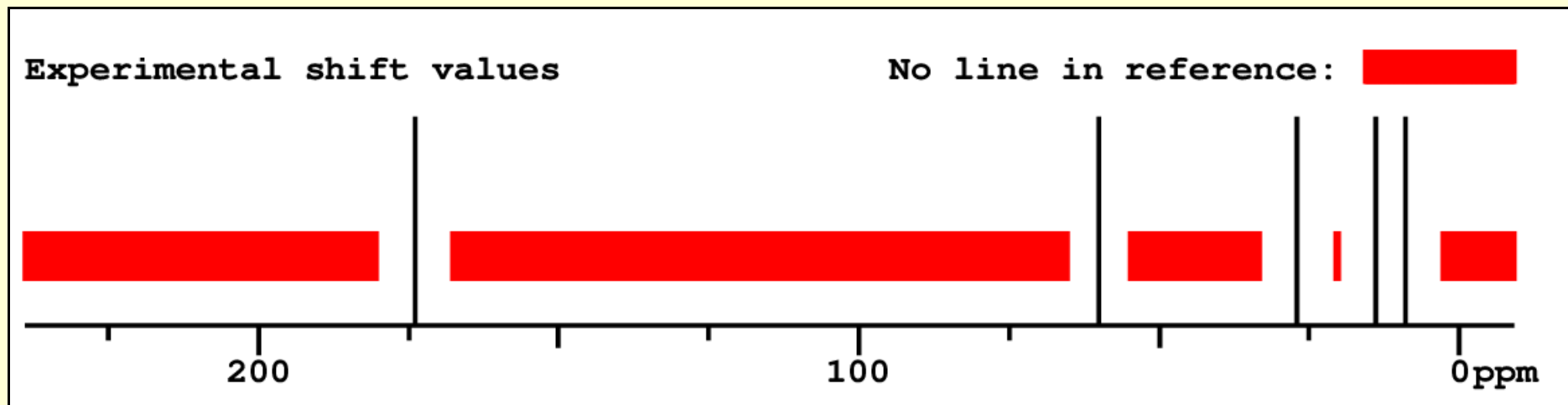
This page will be kept for 30 days here

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

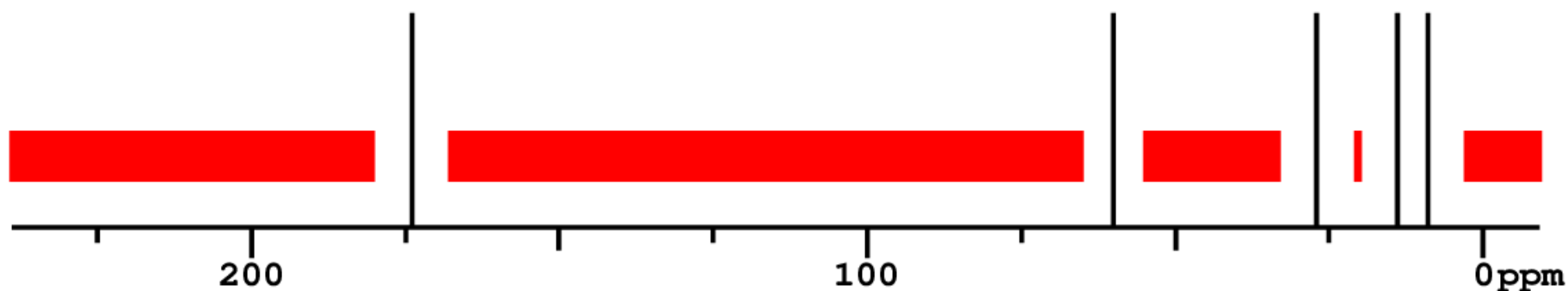
Available entries at each Screening-Step

Total number of entries:	177,099,966
Applying requested elemental composition:	5,102,397 entries remain
Applying requested number of signals:	218,318 entries remain

Entries per line found out of 218,318 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	?	3.00	27,226	Impurity ?
2	60.00	?	2.50	43,893	Unspecific line
3	27.00	?	3.00	73,749	Unspecific line
4	14.00	?	3.00	48,852	Unspecific line
5	9.00	?	3.00	29,238	Unspecific line

Experimental shift values

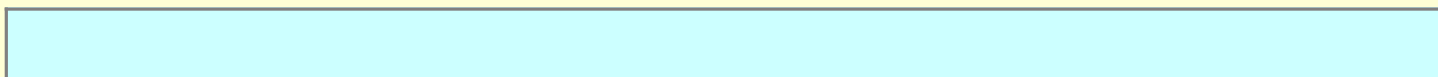
No line in reference: 



Number of coincident lines versus number of entries

Number of coincident lines 5 Lines given	Number of entries	Further Processing
5	96	Selected for detailed analysis
4	1,495	Selected for detailed analysis
3	11,718	
2	45,186	
1	90,972	

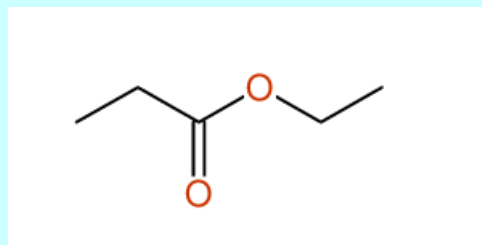
Best 16 Proposals shown for Compound: Propionic_acid,ethylester::400MHz



0.81 -
0.87ppm

3x found

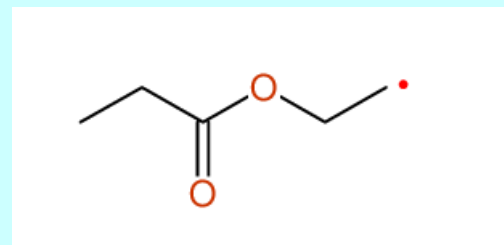
[FKRCODPIKNYEAC](#)



0.81 -
0.81ppm

1x found

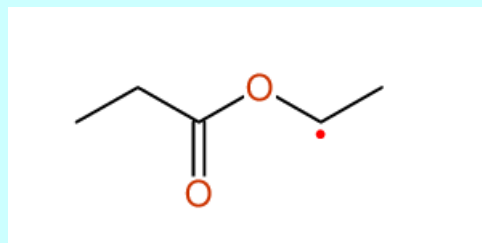
[IRGLFRDZYNBBCO](#)



0.87 -
0.87ppm

1x found

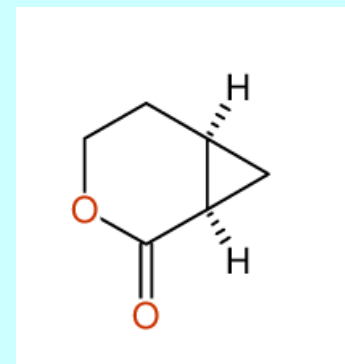
[JLCVJT LAUOPPEG](#)



1.75 -
1.75ppm

1x found

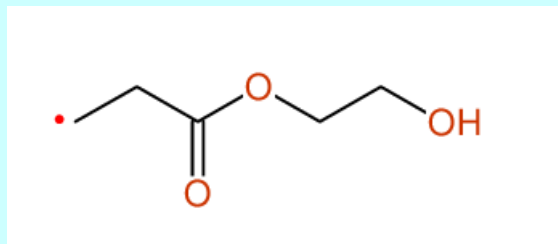
[SSRGPASETRMVON](#)



2.02 -
2.02ppm

1x found

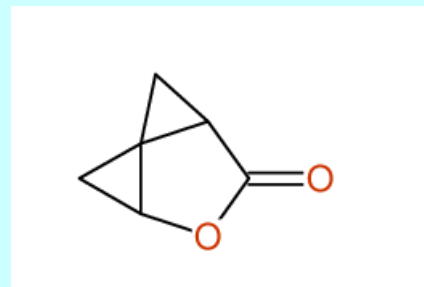
[SRWDELNQQOGFGE](#)



2.85 -
2.85ppm

1x found

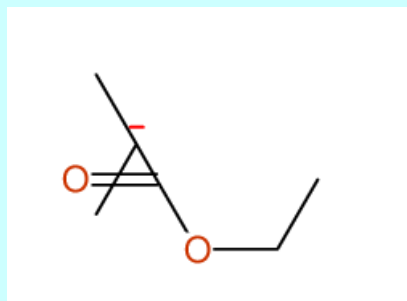
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2.93 -
2.93ppm

1x found

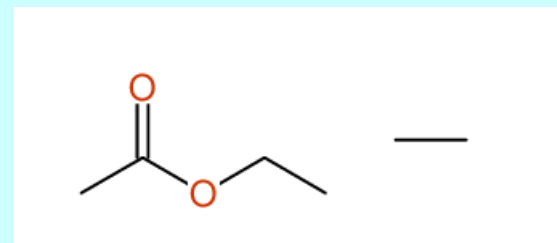
[VNCTWNKFZURVGE](#)



3.27 -
3.27ppm

1x found

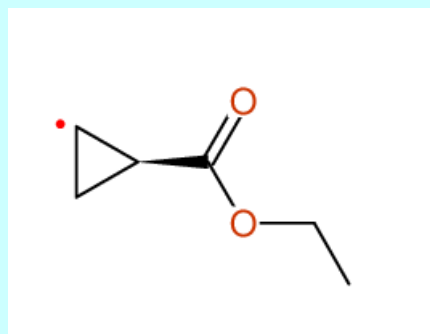
[ZRKANPPNISQQGA](#)



3.30 -
3.30ppm

4x found

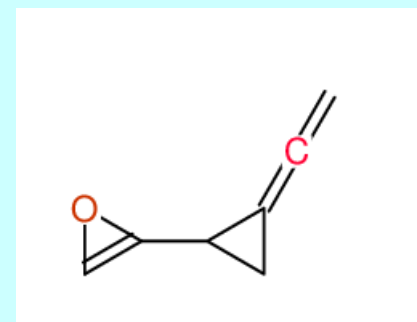
[XJFUMKLBHKVVOM](#)



3.63 -
3.63ppm

1x found

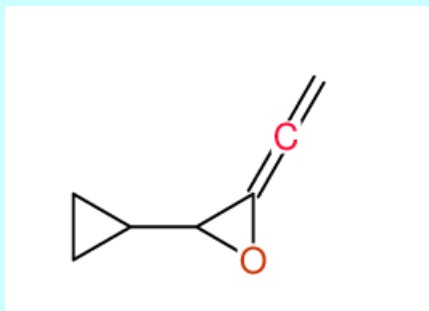
[SIOSIFTVQXCKHE](#)



3.98 -
3.98ppm

1x found

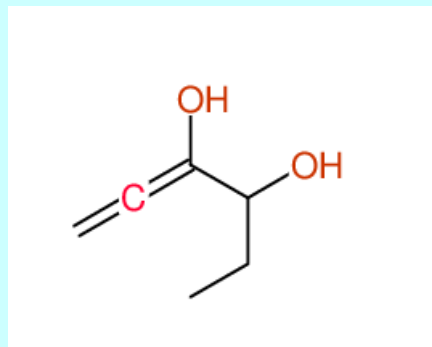
[SQWBZVNZMXUDFY](#)



4.72 -
4.72ppm

1x found

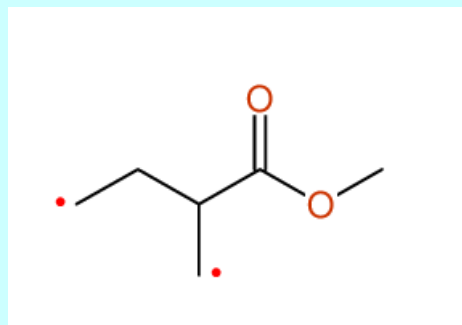
[BIFODGMOCCJWOI](#)



5.25 -
5.25ppm

1x found

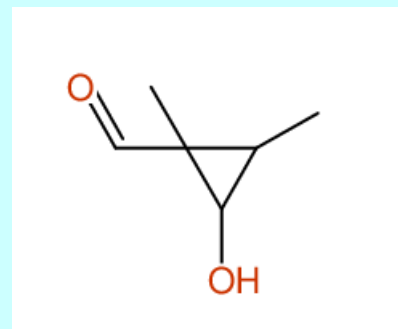
[YTEGYFGYGIPBPK](#)



5.61 -
5.61ppm

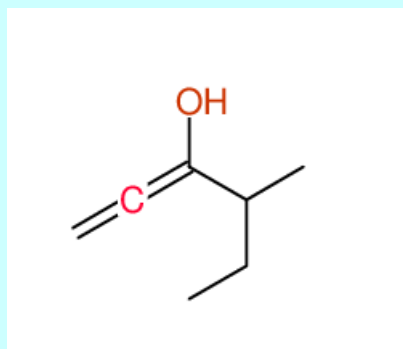
1x found

[HIHLRSKFLUZMEZ](#)

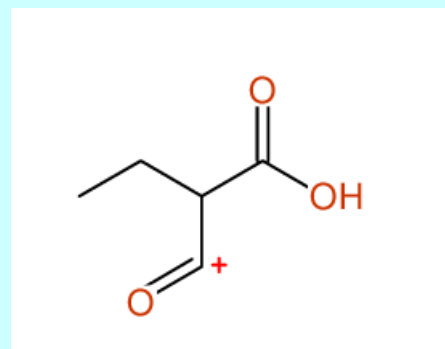


6.01 -
6.01ppm

1x found

[VNLWRJLKFXZXXCL](#)8.84 -
9.70ppm

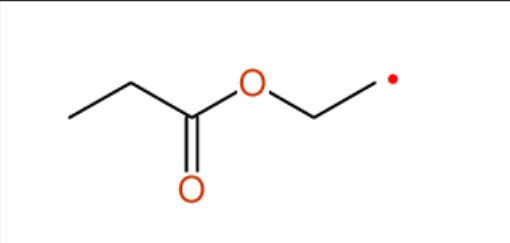
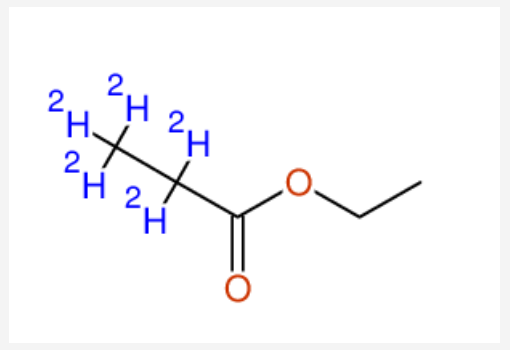
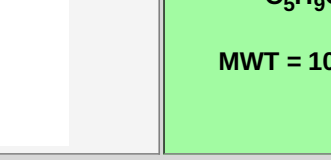
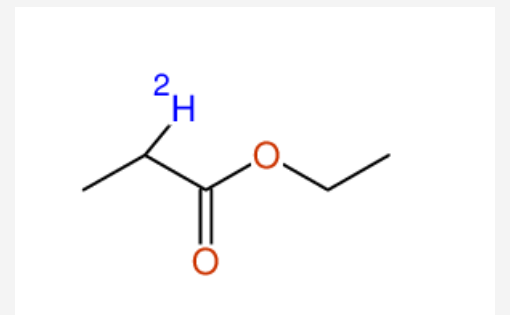

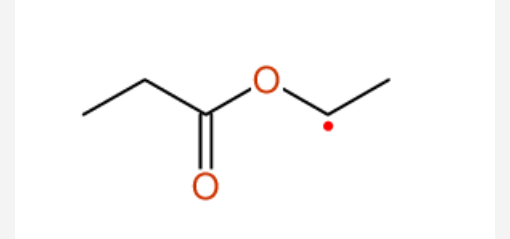
2x found

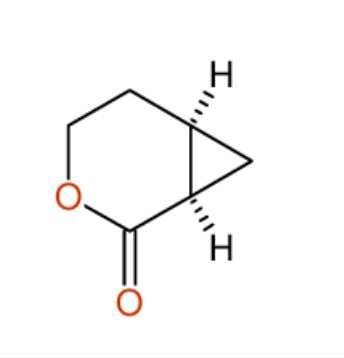
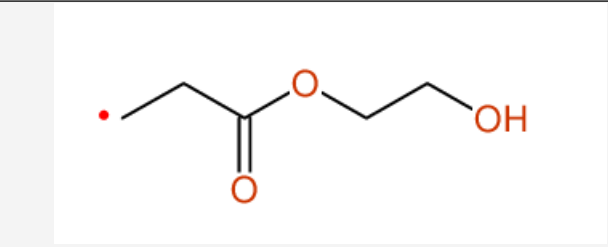
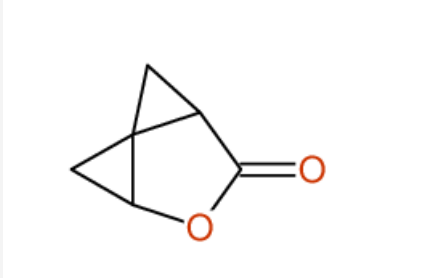
[XKQXOPMMXGTFOA](#)

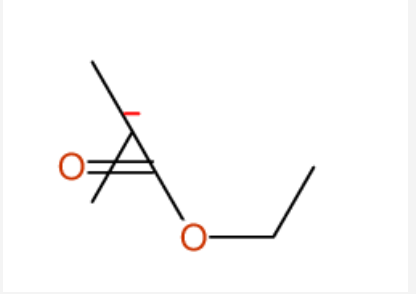
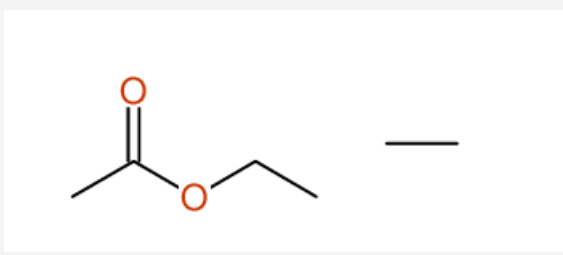
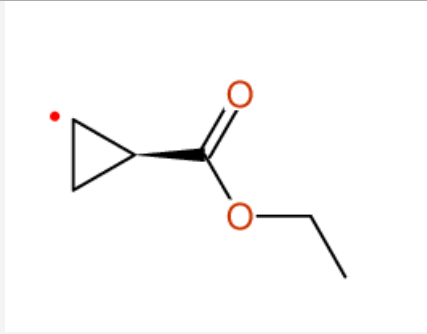
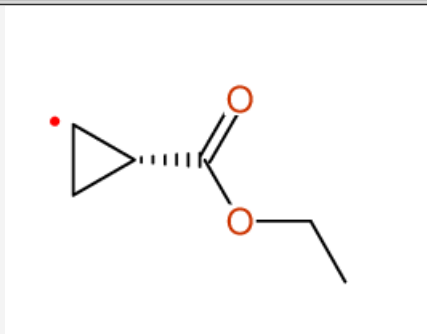
1,591 [Structure proposals](#) found for your C-NMR Spectrum

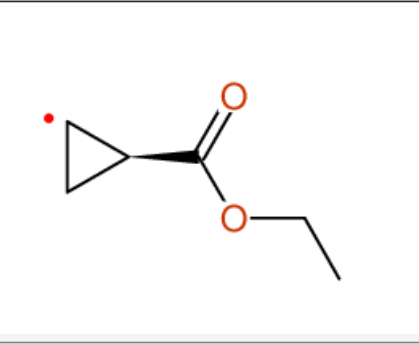
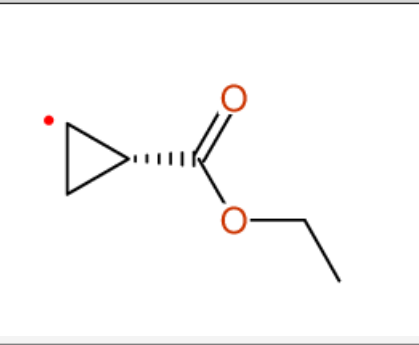
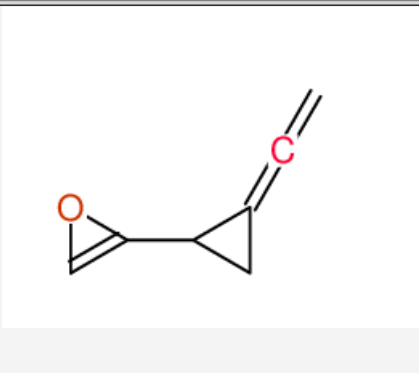
70 Entries will be shown because of your selection of additional constraints

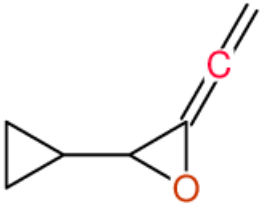
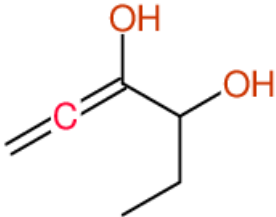
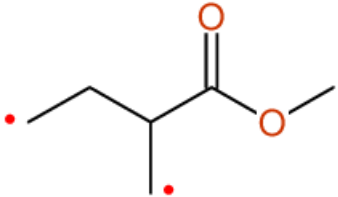
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #1 0.81 Details		$C_5H_{10}O_2$ MWT = 102.055	Proposal #1 Structure-ID: 6,776,925 FKRCODPIKNYEAC-IKLDFFBCSAQ	Availability of NMR-Data in CSEARCH

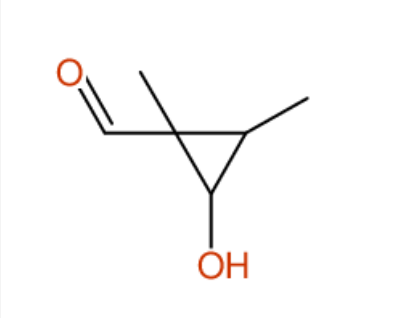
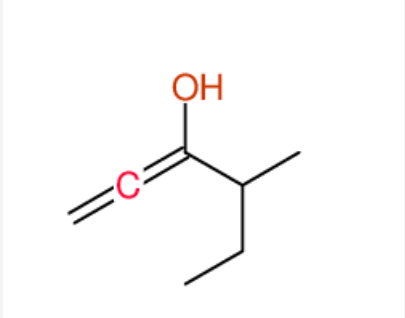
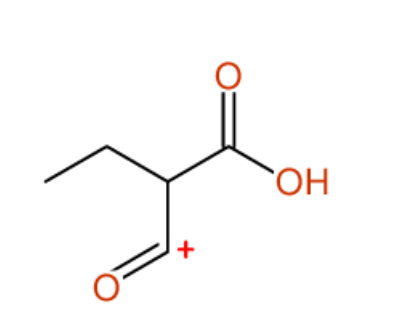
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #2 0.81 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #2 Structure-ID: 6,773,007 IRGLFRDZYNBBCO-IKLDIFBCSAI	
Proposal #3 0.87 Details		$C_5H_{10}O_2$ MWT = 107.055	Proposal #3 Structure-ID: 27,004,293 FKRCODPIKNYEAC-WNWXXORZEL	Availability of NMR-Data in CSEARCH 
Proposal #4 0.87 Details		$C_5H_{10}O_2$ MWT = 103.055	Proposal #4 Structure-ID: 77,343,682 FKRCODPIKNYEAC-WFVSECRTEI	Availability of NMR-Data in CSEARCH 
Proposal #5 0.87 Details		$C_5H_{10}O_2$ MWT = 101.055	Proposal #5 Structure-ID: 35,970,584 JLCVJT LAUOPPF G-UHFFFAOYAG	

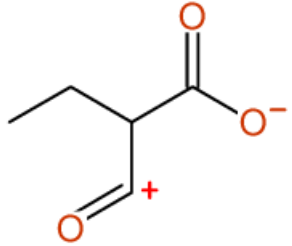
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #6</p> <p>1.75</p> <p>Details</p>		<p>$C_6H_8O_2$</p> <p>MWT = 112.066</p>	<p>Proposal #6</p> <p>Structure-ID: 35,744,386</p> <p>SSRGPASETRMVON-CRCLSJGQBP</p>	
<p>Proposal #7</p> <p>2.02</p> <p>Details</p>		<p>$C_5H_9O_3$</p> <p>MWT = 117.055</p>	<p>Proposal #7</p> <p>Structure-ID: 35,385,805</p> <p>SRWDELNQQOGFGE-UHFFFAOYAC</p>	
<p>Proposal #8</p> <p>2.85</p> <p>Details</p>		<p>$C_6H_6O_2$</p> <p>MWT = 110.066</p>	<p>Proposal #8</p> <p>Structure-ID: 157,622,171</p> <p>WZLNCRVWIKHJER-UHFFFAOYAF</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #9 2.93 Details		$C_6H_{11}O_2$ MWT = 115.066	Proposal #9 Structure-ID: 132,225,892 VNCTWNKFZURVGF-UHFFFAOYAA	
Proposal #10 3.27 Details Different pattern		$C_4H_8O_2.C_2H_6$ MWT = 118.066	Proposal #10 Structure-ID: 12,183,409 ZRKANPPNISQQGA-UHFFFAOYAP	
Proposal #11 3.30 Details		$C_6H_9O_2$ MWT = 113.066	Proposal #11 Structure-ID: 35,252,528 XJFUMKLBHKVVOM-RXMQYKEDBB	
Proposal #12 3.30 Details		$C_6H_9O_2$ MWT = 113.066	Proposal #12 Structure-ID: 35,252,530 XJFUMKLBHKVVOM-YFKPBYRBJ	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #13</p> <p>3.30</p> <p>Details</p>		<p>$C_6H_9O_2$</p> <p>MWT = 113.066</p>	<p>Proposal #13</p> <p>Structure-ID: 35,036,550</p> <p>XJFUMKLBHKVVOM-RXMQYKEDBB</p>	
<p>Proposal #14</p> <p>3.30</p> <p>Details</p>		<p>$C_6H_9O_2$</p> <p>MWT = 113.066</p>	<p>Proposal #14</p> <p>Structure-ID: 35,036,552</p> <p>XJFUMKLBHKVVOM-YFKPBYRVBJ</p>	
<p>Proposal #15</p> <p>3.63</p> <p>Details</p>		<p>C_7H_6O</p> <p>MWT = 106.077</p>	<p>Proposal #15</p> <p>Structure-ID: 146,798,417</p> <p>SIOSIFTVQXCKHF-UHFFFAOYAV</p>	

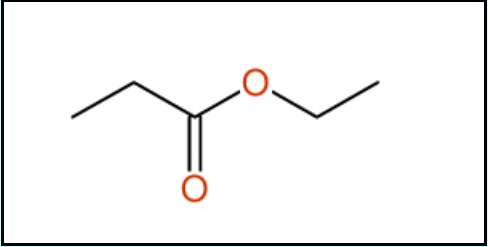
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #16</p> <p>3.98</p> <p>Details</p>		<p>C_7H_8O</p> <p>MWT = 108.077</p>	<p>Proposal #16</p> <p>Structure-ID: 146,798,687</p> <p>SQWBZVNZMXUDFY-UHFFFAOYAX</p>	
<p>Proposal #17</p> <p>4.72</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #17</p> <p>Structure-ID: 157,518,290</p> <p>BIFODGMOCCJWOI-UHFFFAOYAP</p>	
<p>Proposal #18</p> <p>5.25</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #18</p> <p>Structure-ID: 28,087,785</p> <p>YTEGYFGYGIPBPK-UHFFFAOYAM</p>	

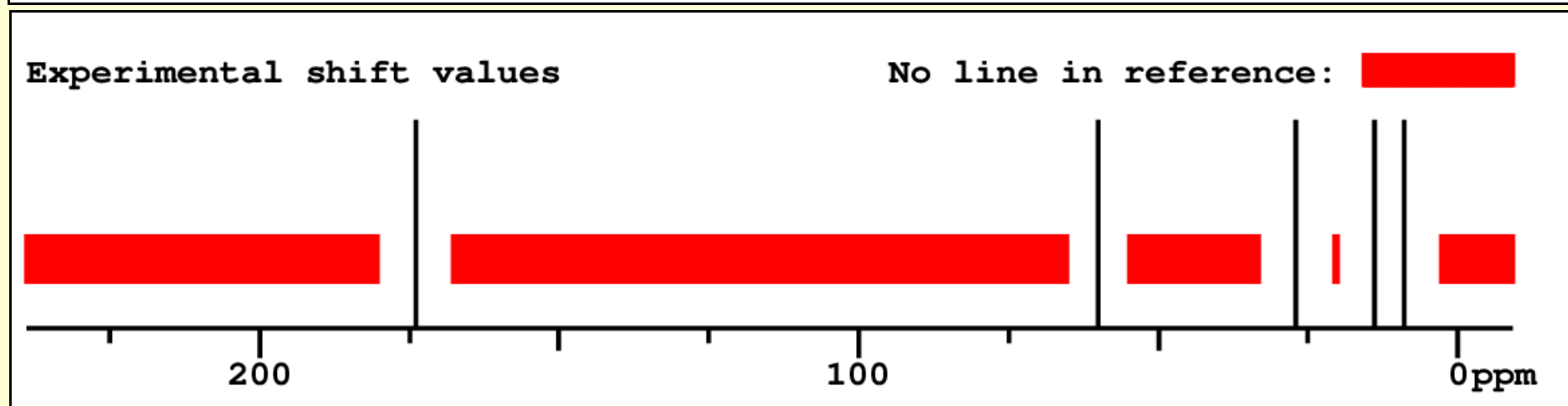
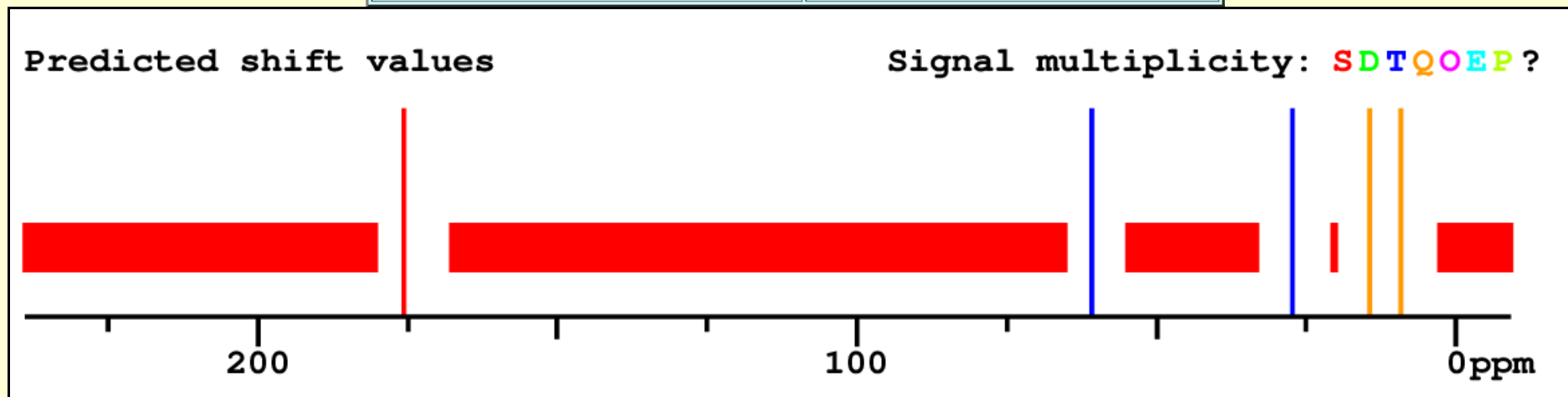
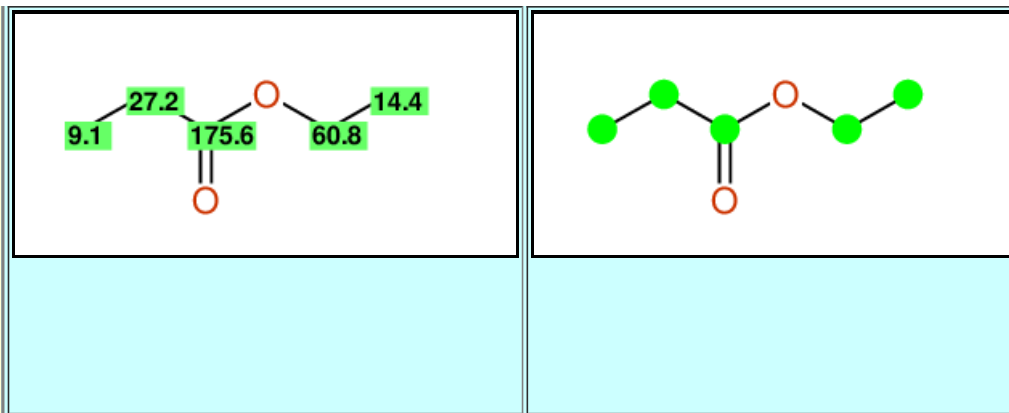
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
<p>Proposal #19</p> <p>5.61</p> <p>Details</p> <p>Different pattern</p>		<p>$C_6H_{10}O_2$</p> <p>MWT = 114.066</p>	<p>Proposal #19</p> <p>Structure-ID: 157,727,304</p> <p>HIHLRSKFLUZMFZ-UHFFFAOYAO</p>	
<p>Proposal #20</p> <p>6.01</p> <p>Details</p> <p>Different pattern</p>		<p>$C_7H_{12}O$</p> <p>MWT = 112.077</p>	<p>Proposal #20</p> <p>Structure-ID: 157,518,275</p> <p>VNLWRJLKFZXXCL-UHFFFAOYAE</p>	
<p>Proposal #21</p> <p>8.84</p> <p>Details</p>		<p>$C_5H_6O_3$</p> <p>MWT = 114.055</p>	<p>Proposal #21</p> <p>Structure-ID: 66,560,737</p> <p>XKQXOPMMXGTFOA-IKLD FBCSAL</p>	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
Proposal #22 9.70 Details		$C_5H_6O_3$ MWT = 114.055	Proposal #22 Structure-ID: 66,560,736 XKQXOPMMXGTFOA-UHFFFAOYAR	

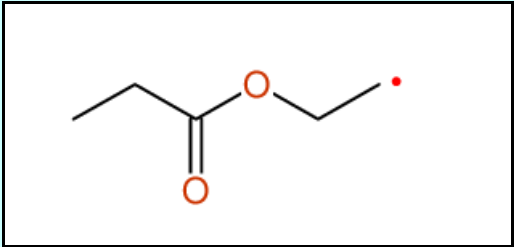
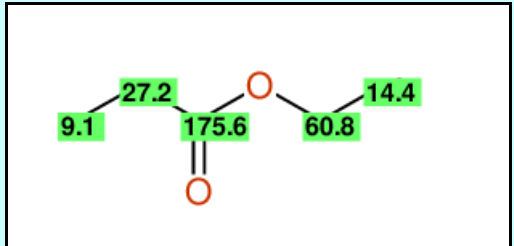
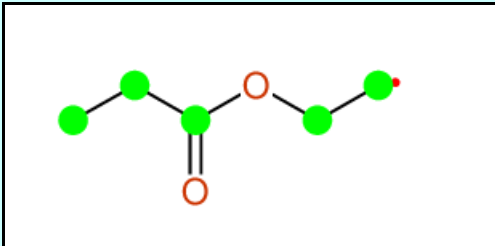
Detailed Analysis

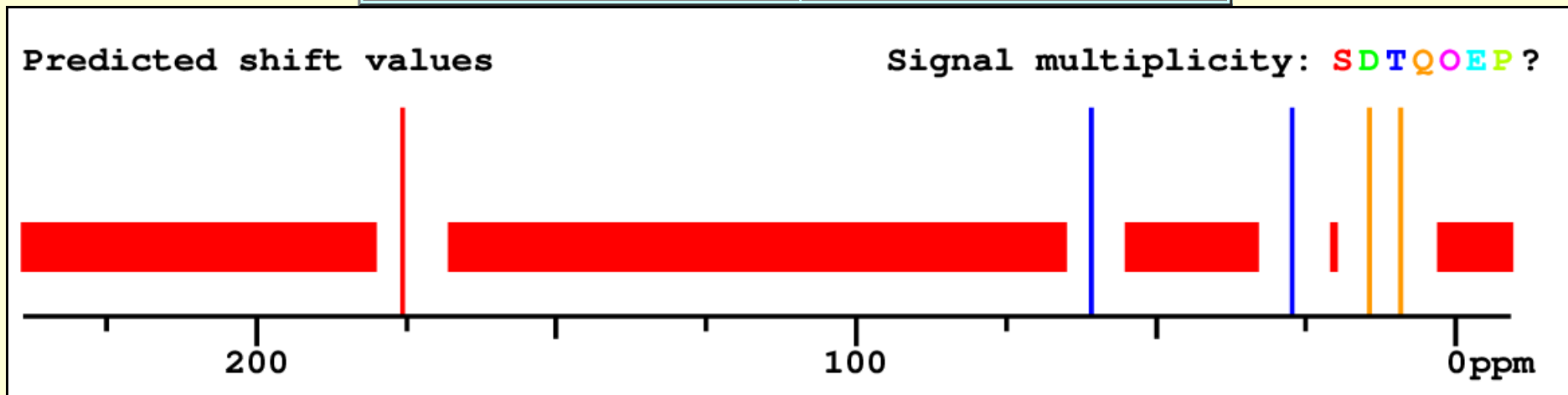
Structure Proposal #1

Structure	Similarity Measure
	Deviation = 0.81 ppm Similarity = 100 % $C_5H_{10}O_2$ MWT = 102.06 Search Web for this structure: FKRCODPIKNYEAC Availability
Predicted Chemical Shiftvalues	Matching Map




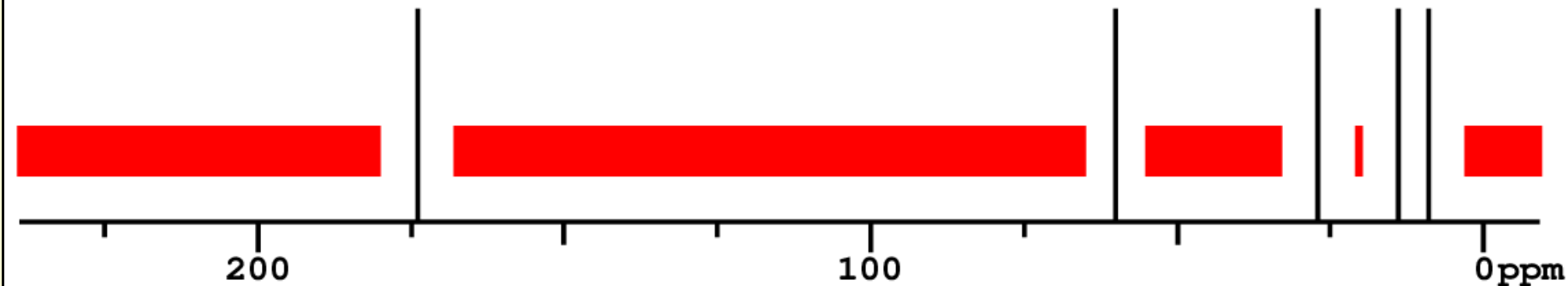
Structure Proposal #2

Structure	Similarity Measure
	Deviation = 0.81 ppm Similarity = 100 % C ₅ H ₉ O ₂ MWT = 101.06 Search Web for this structure: IRGLFRDZYNBBCO
Predicted Chemical Shiftvalues	Matching Map
	



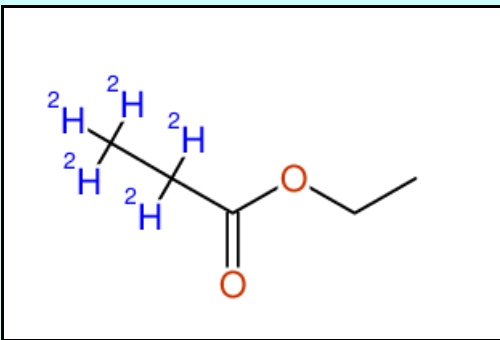
Experimental shift values

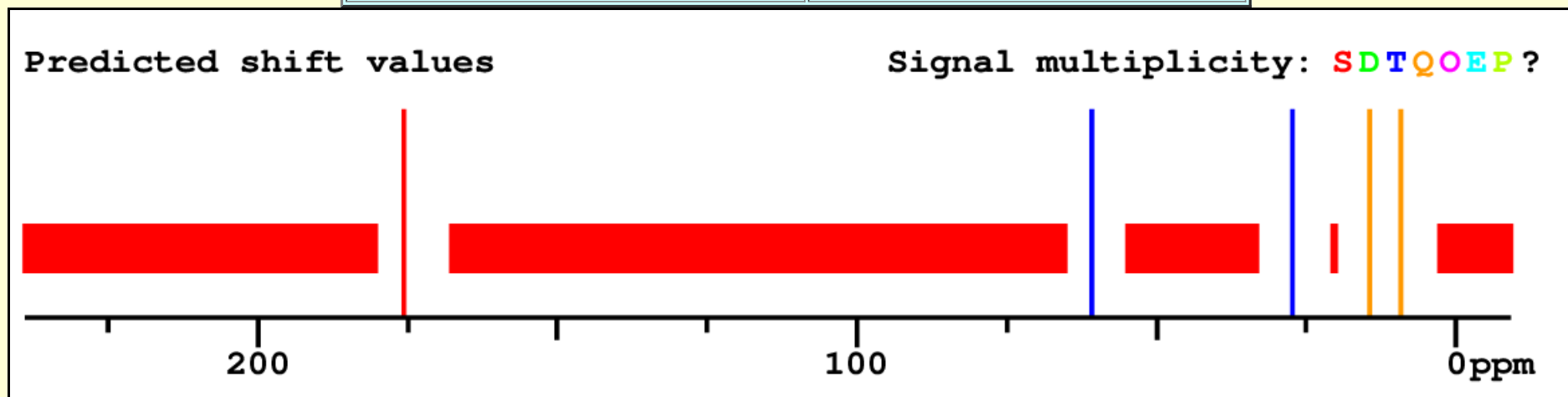
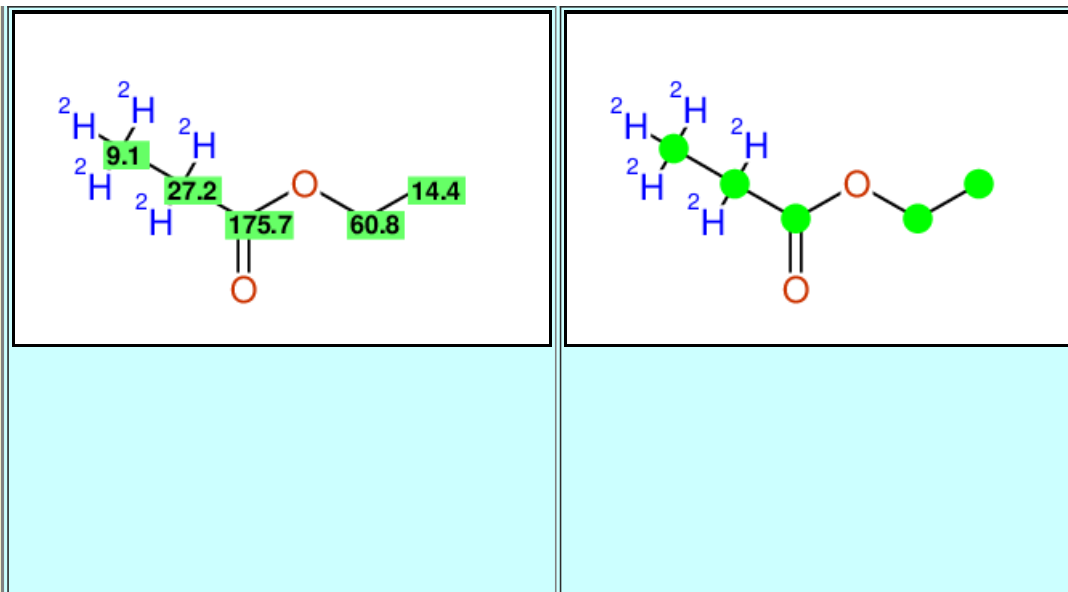
No line in reference: 




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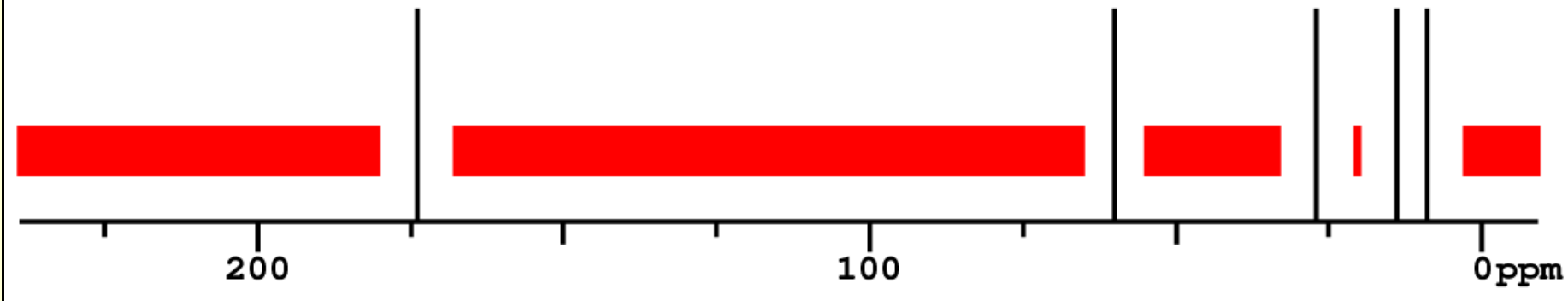
Structure Proposal #3

Structure	Similarity Measure
	Deviation = 0.87 ppm Similarity = 100 % C ₅ H ₁₀ O ₂ MWT = 107.06 Search Web for this structure: FKRCODPIKNYEAC Availability
Predicted Chemical Shiftvalues	Matching Map



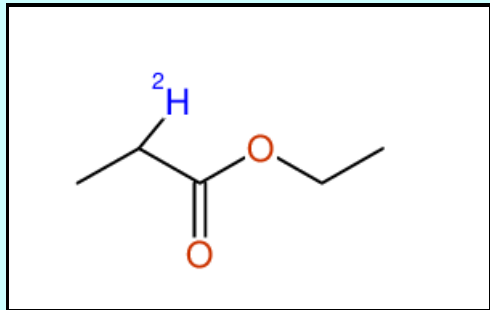
Experimental shift values

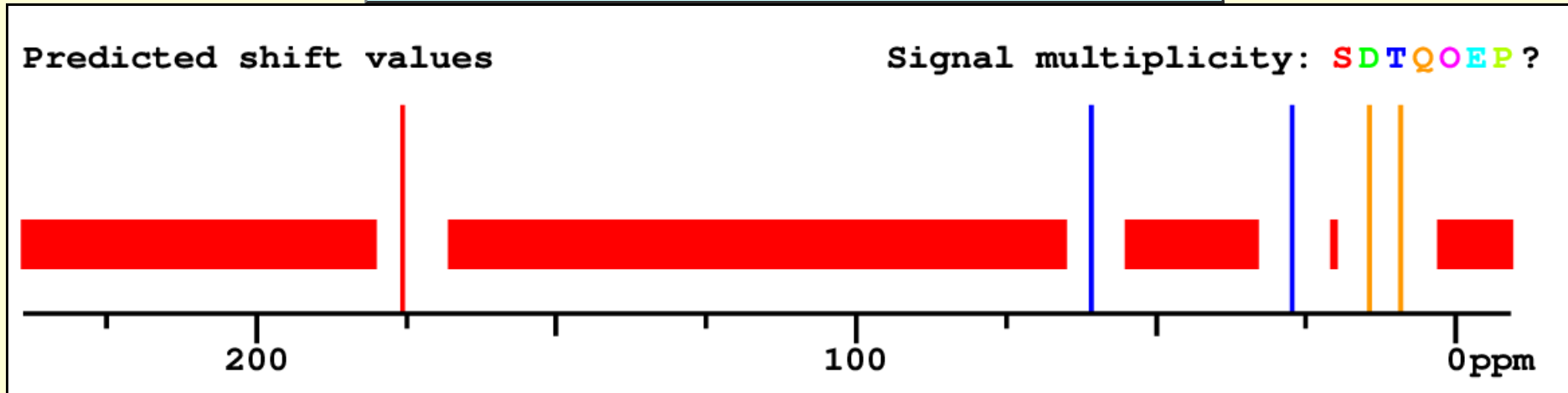
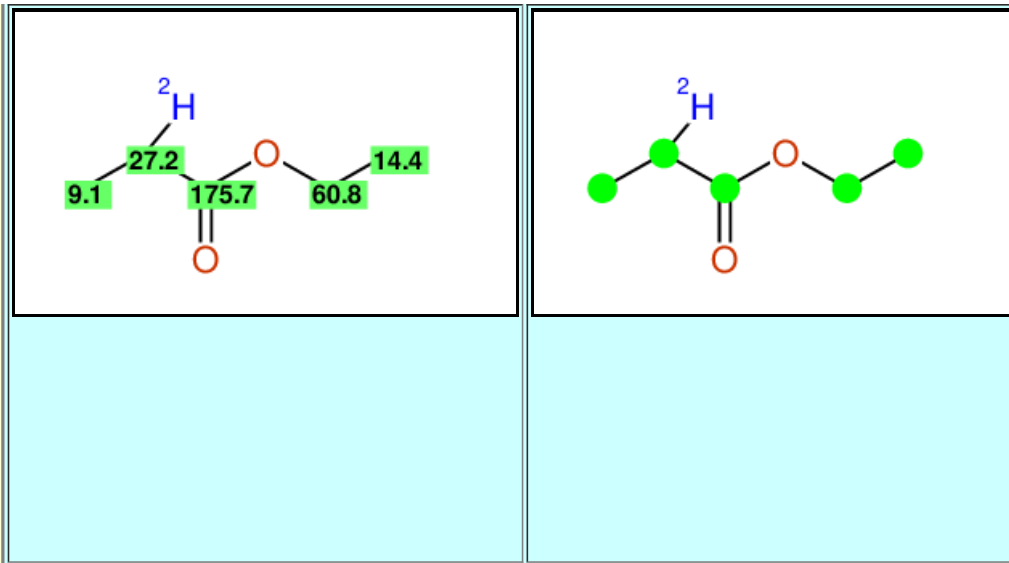
No line in reference: 



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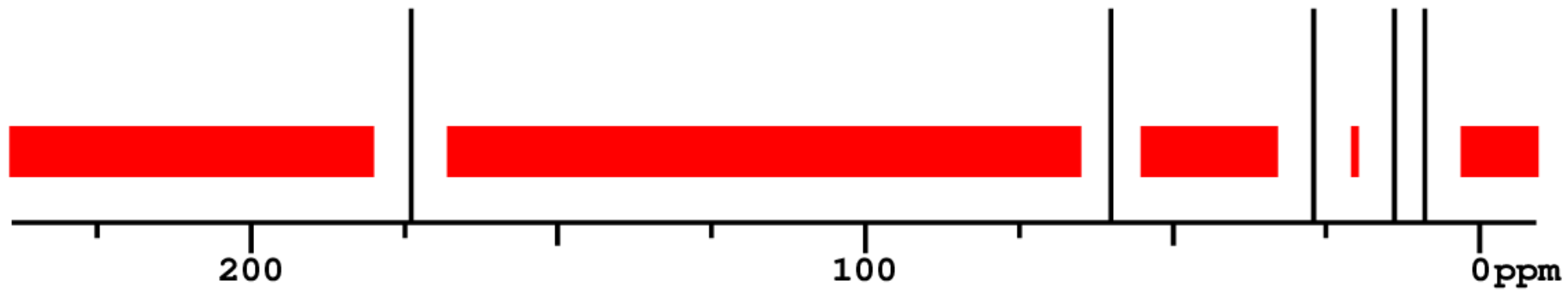
Structure Proposal #4

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



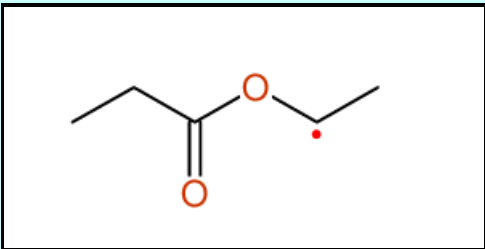
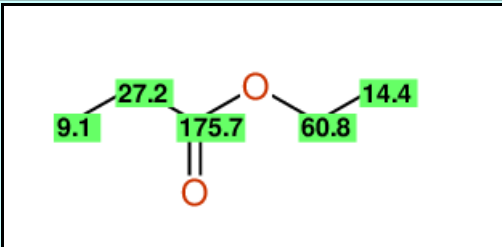
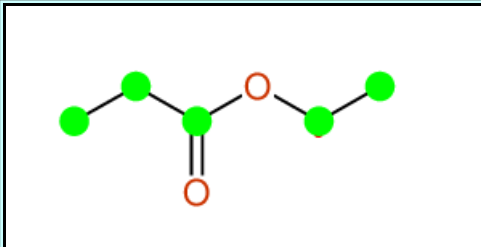
Experimental shift values

No line in reference: 



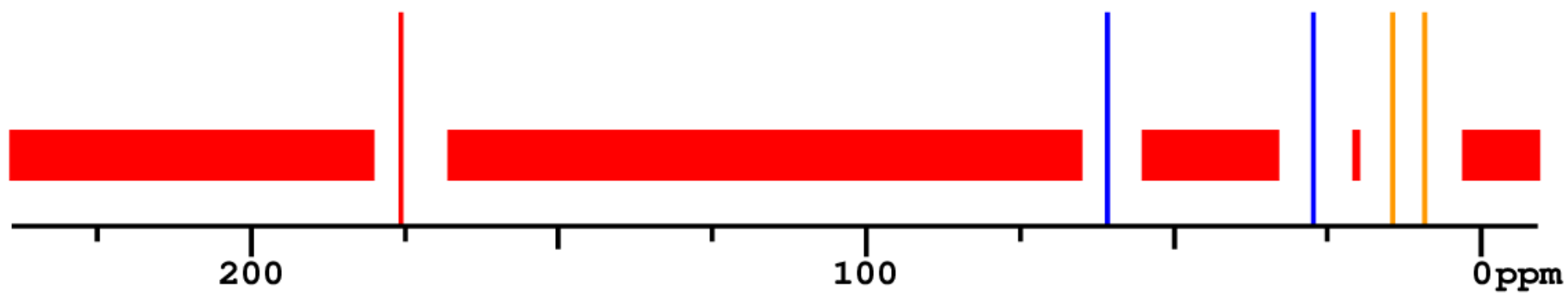
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Structure Proposal #5

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

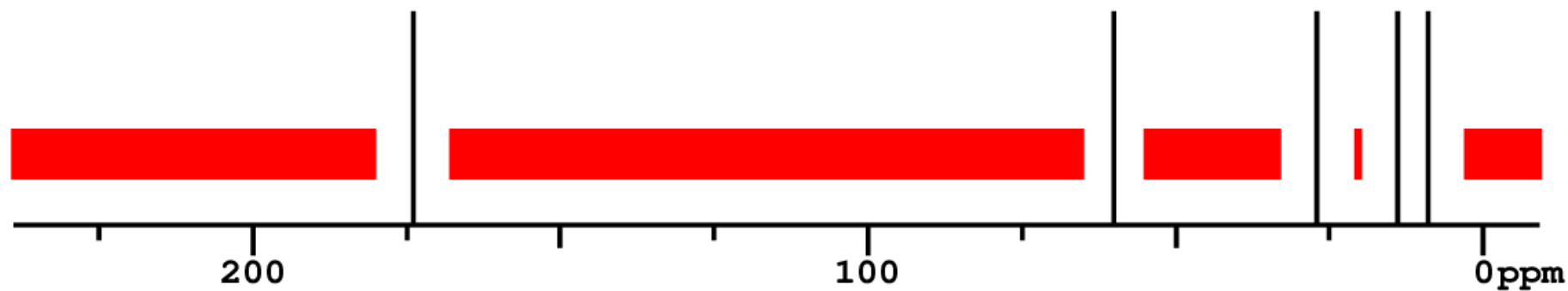
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

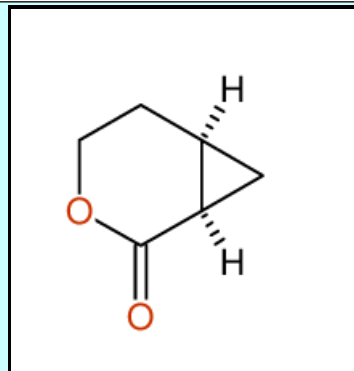
No line in reference: [red bar]



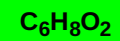
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Structure Proposal #6

Structure	Similarity Measure



Deviation = 1.75 ppm
Similarity = 92 %

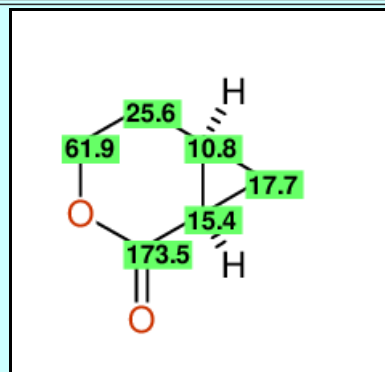


MWT = 112.07

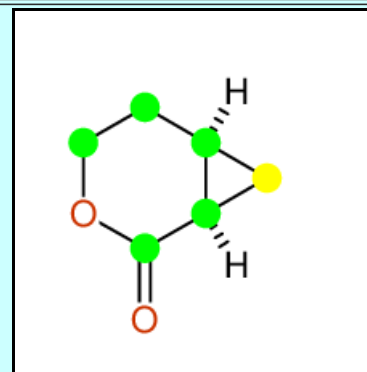
Search Web for this
structure:

[SSRGPASETRMVON](#)

Predicted Chemical
Shiftvalues

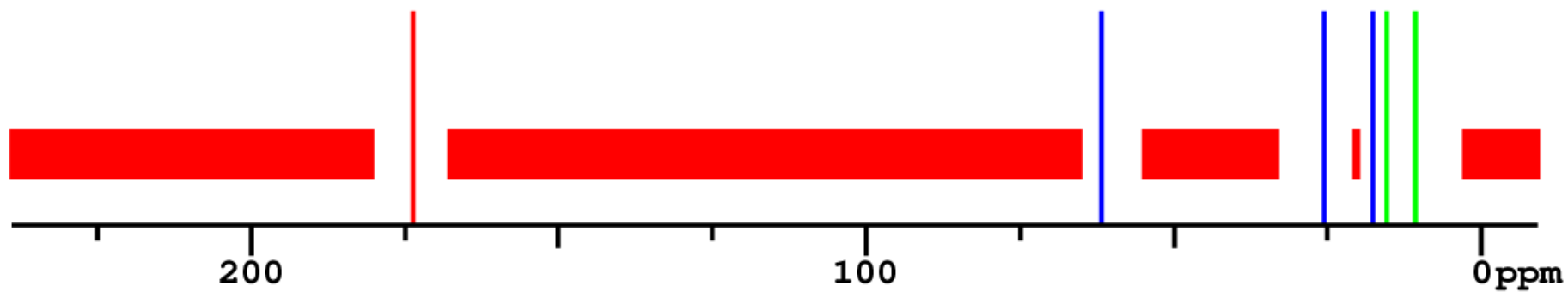


Matching Map



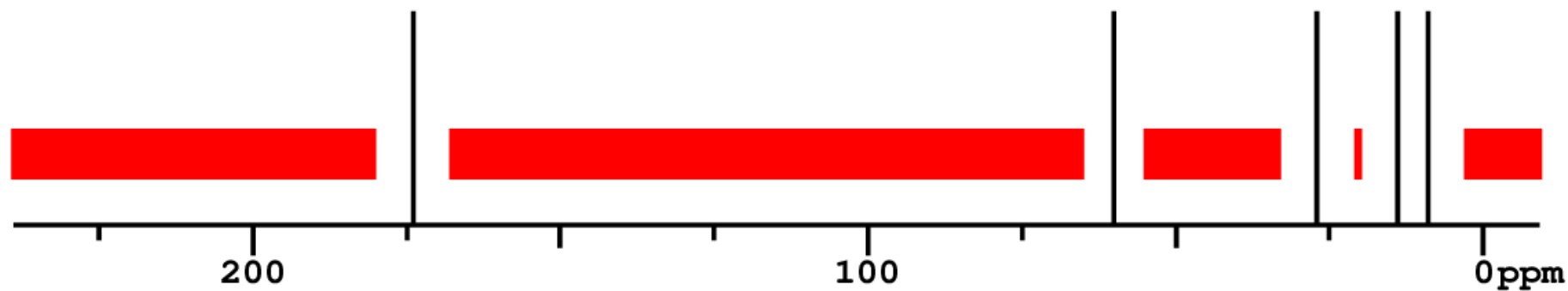
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

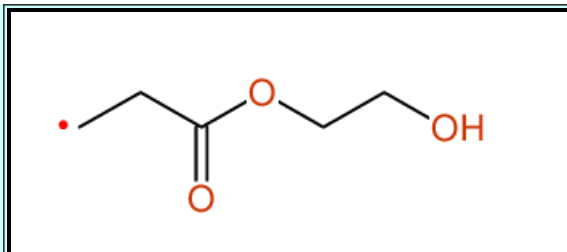
No line in reference: [red bar]



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Structure Proposal #7

Structure	Similarity Measure



Deviation = 2.02 ppm
Similarity = 90 %

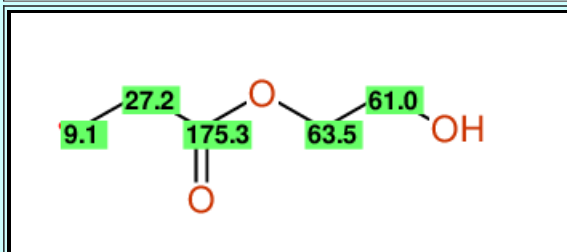
$C_5H_9O_3$

MWT = 117.06

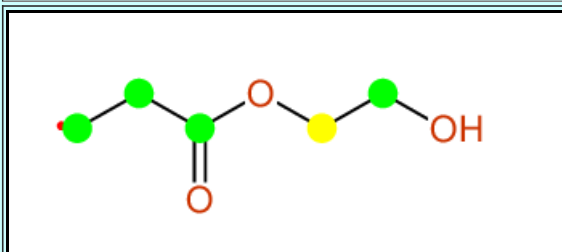
Search Web for this structure:

[SRWDELNQOGFGE](#)

Predicted Chemical Shiftvalues

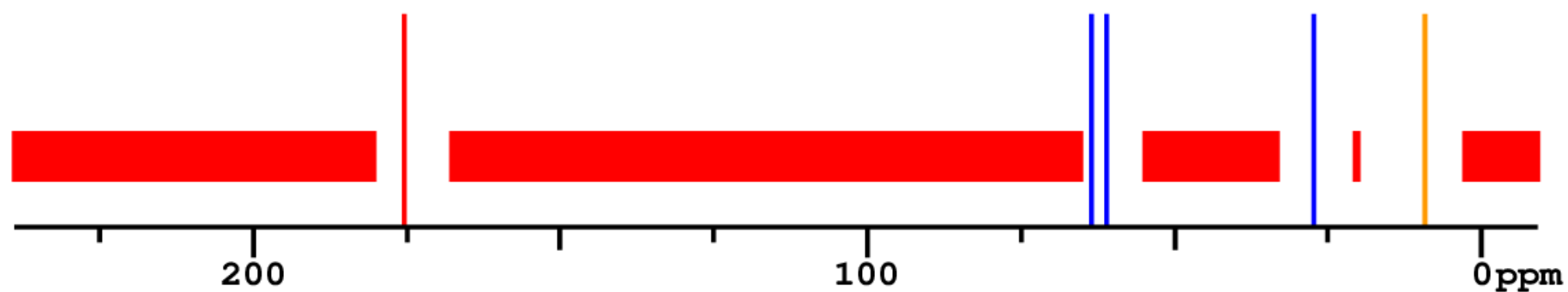


Matching Map



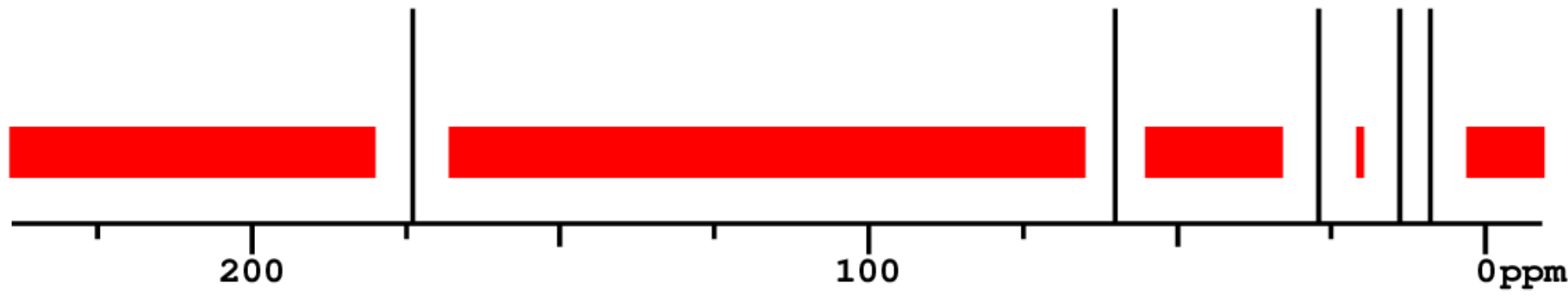
Predicted shift values

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



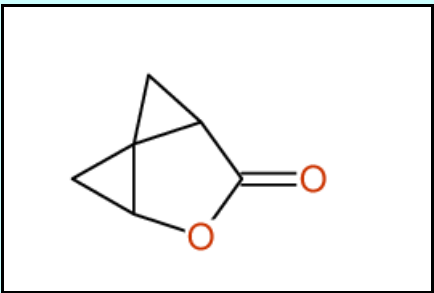
Experimental shift values

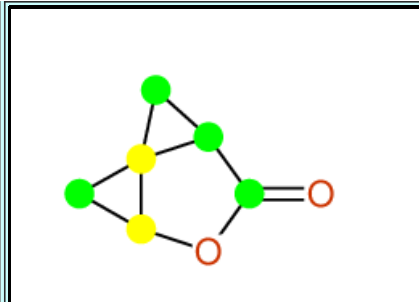
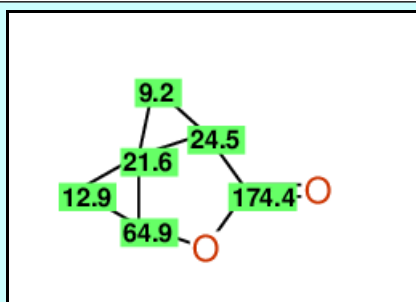
No line in reference: 



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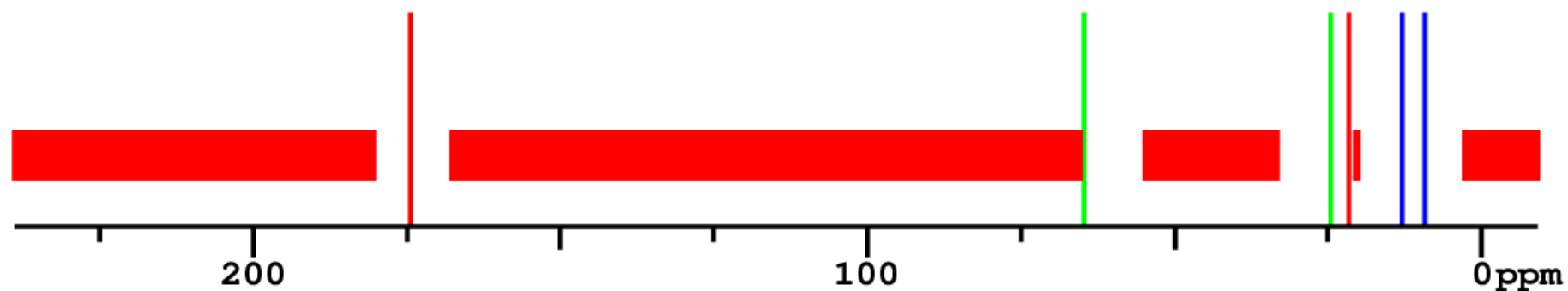
Structure Proposal #8

Structure	Similarity Measure
	Deviation = 2.85 ppm Similarity = 83 % $C_6H_6O_2$ MWT = 110.07 Search Web for this structure: WZLNCRVWIKHJER
Predicted Chemical Shiftvalues	Matching Map



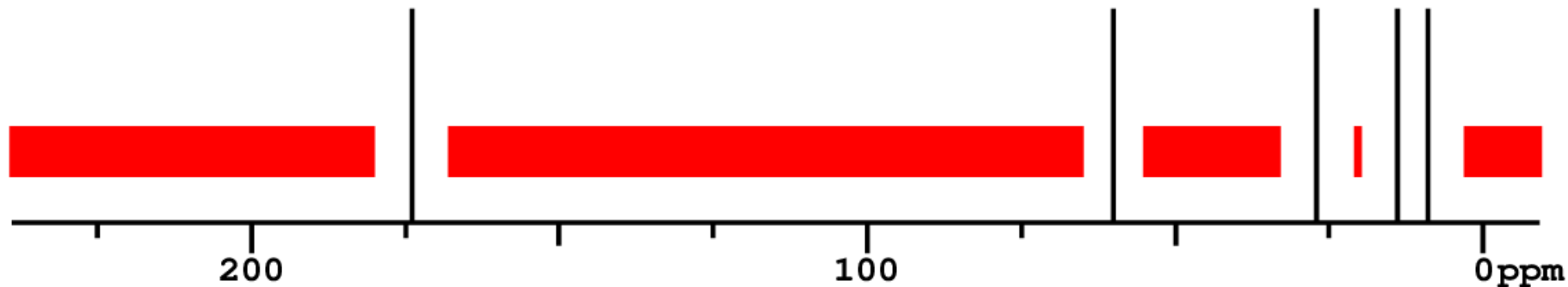
Predicted shift values

Signal multiplicity: S D T Q O E P ?



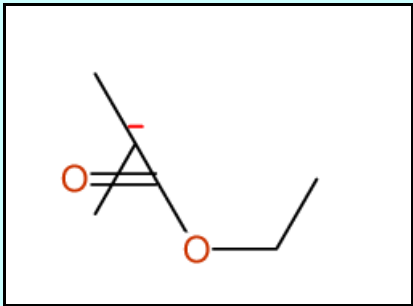
Experimental shift values

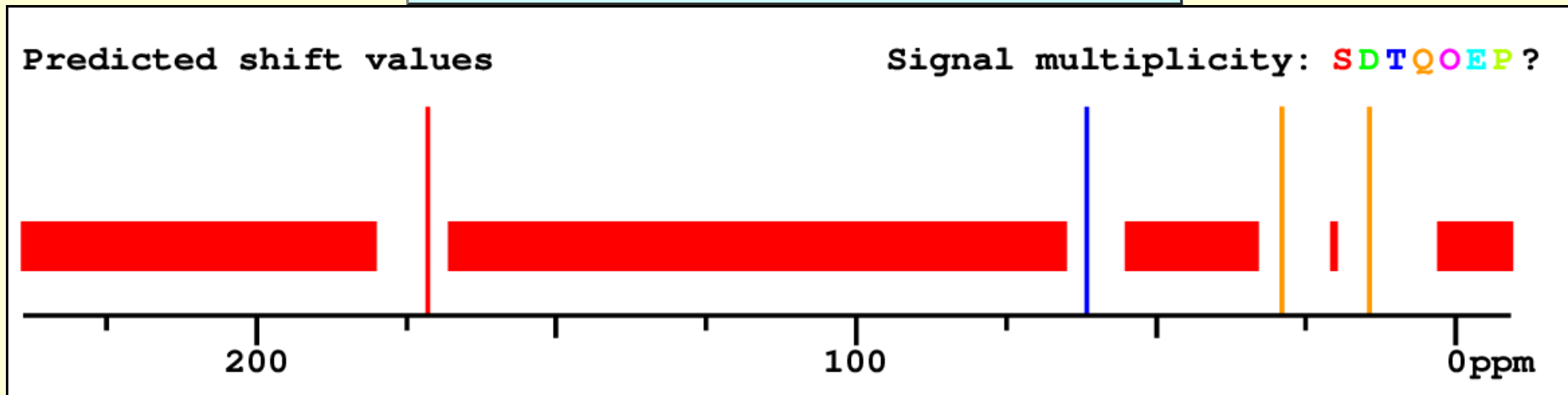
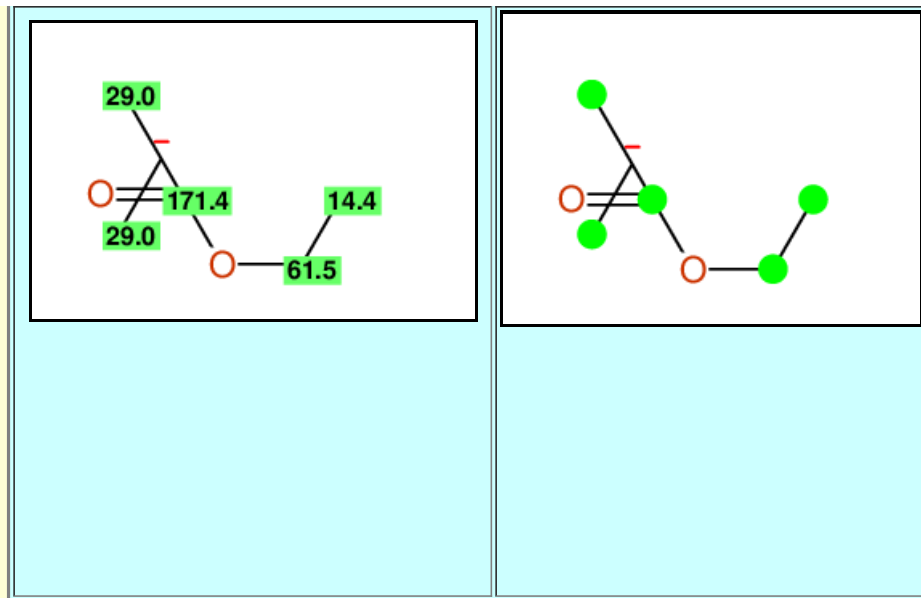
No line in reference: 



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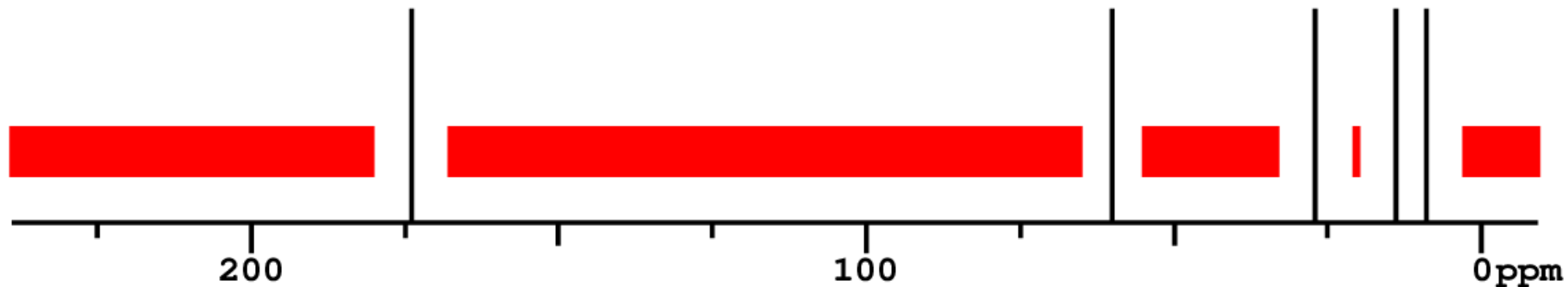
Structure Proposal #9

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



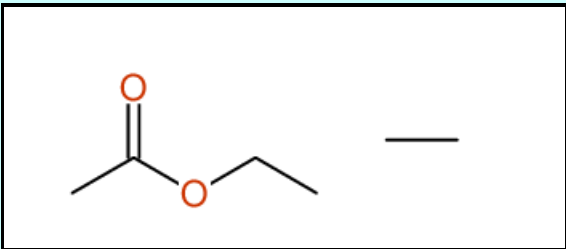
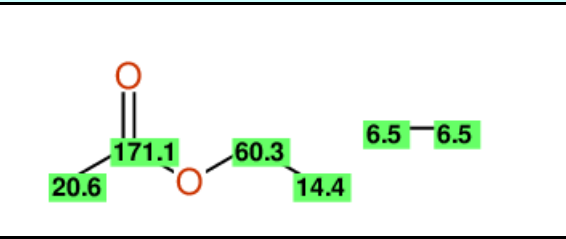
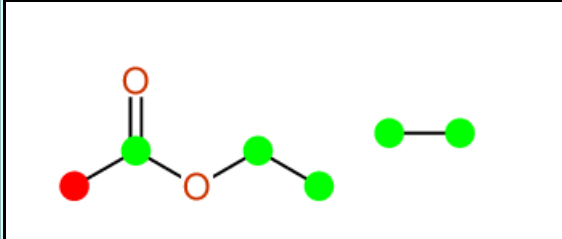
Experimental shift values

No line in reference: ████████



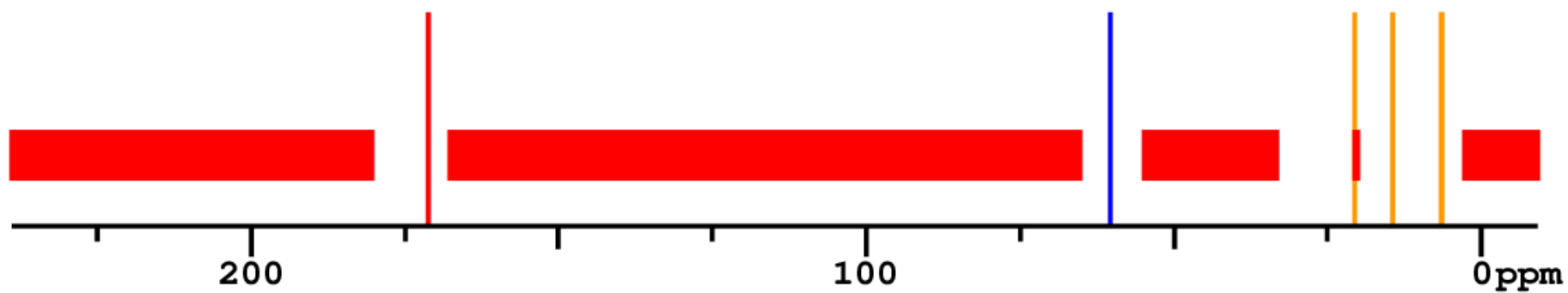
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Structure Proposal #10

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

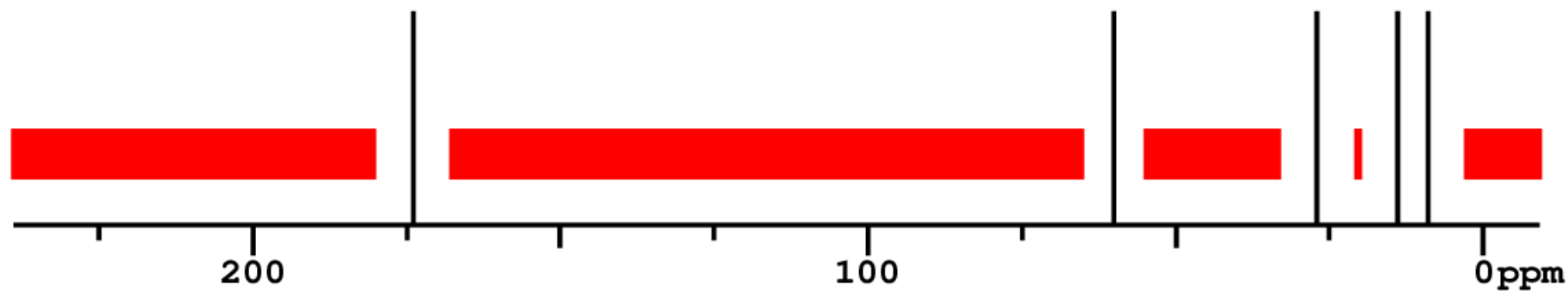
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

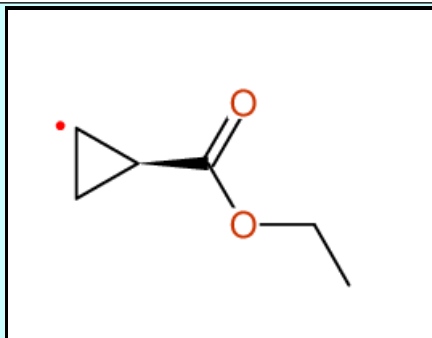
No line in reference: [red bar]



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Structure Proposal #11

Structure	Similarity Measure



Deviation = 3.30 ppm
Similarity = 100 %

$C_6H_9O_2$

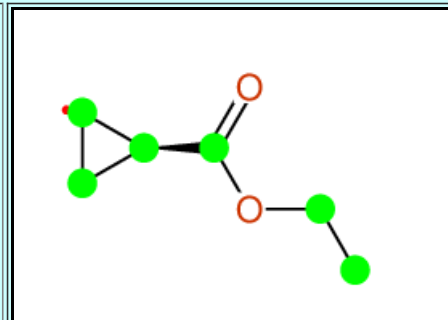
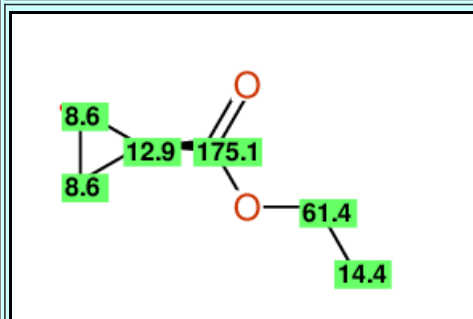
MWT = 113.07

Search Web for this structure:

[XJFUMKLBHKVVOM](#)

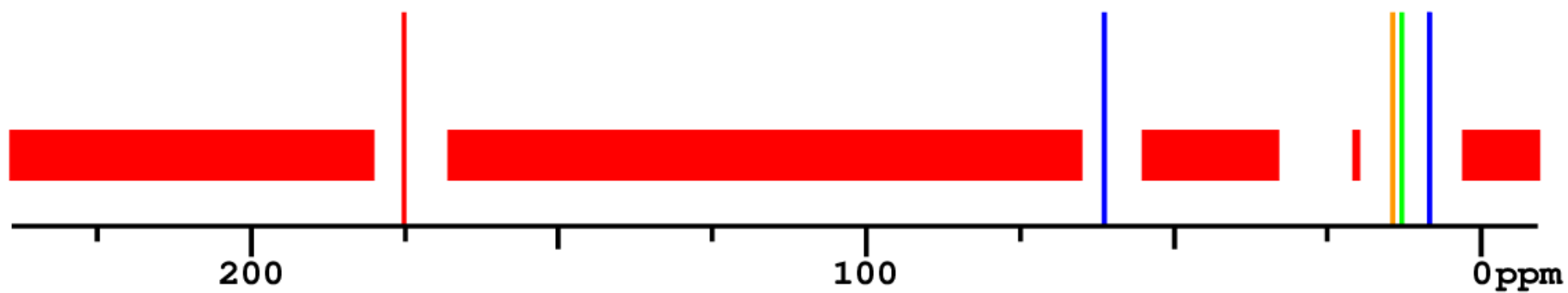
Predicted Chemical Shiftvalues

Matching Map



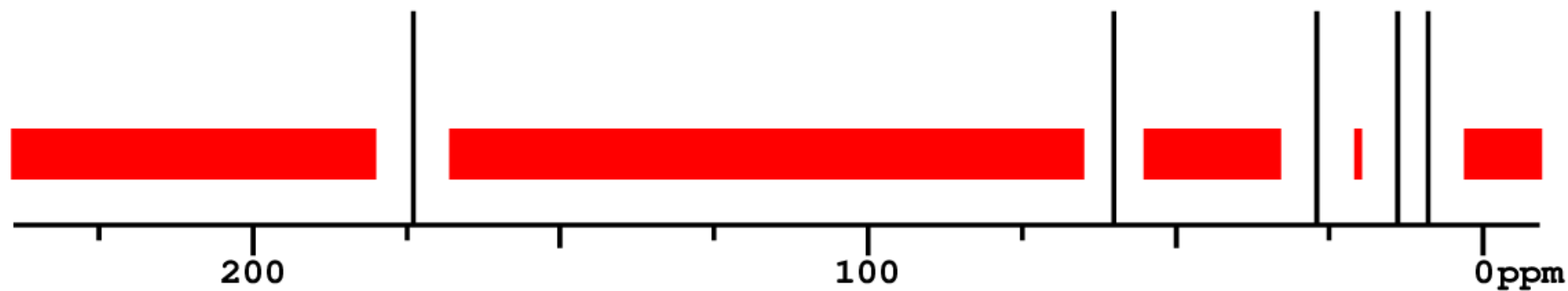
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

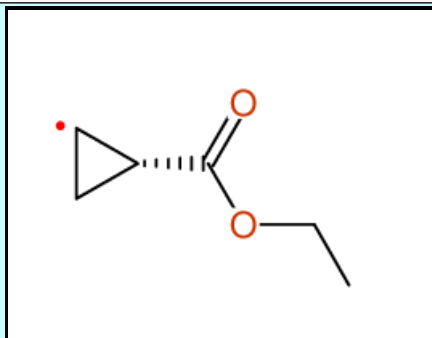
No line in reference: [red bar]



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Structure Proposal #12

Structure	Similarity Measure



Deviation = 3.30 ppm
Similarity = 100 %

$C_6H_9O_2$

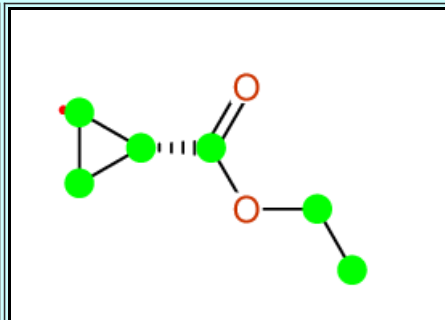
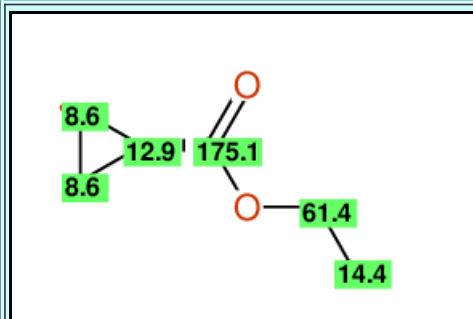
MWT = 113.07

Search Web for this structure:

[XJFUMKLBHKVVOM](#)

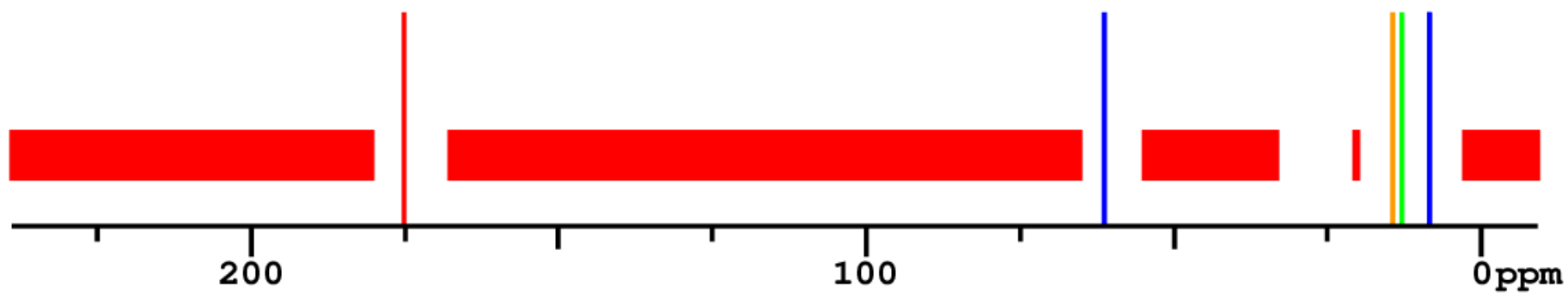
Predicted Chemical Shiftvalues

Matching Map



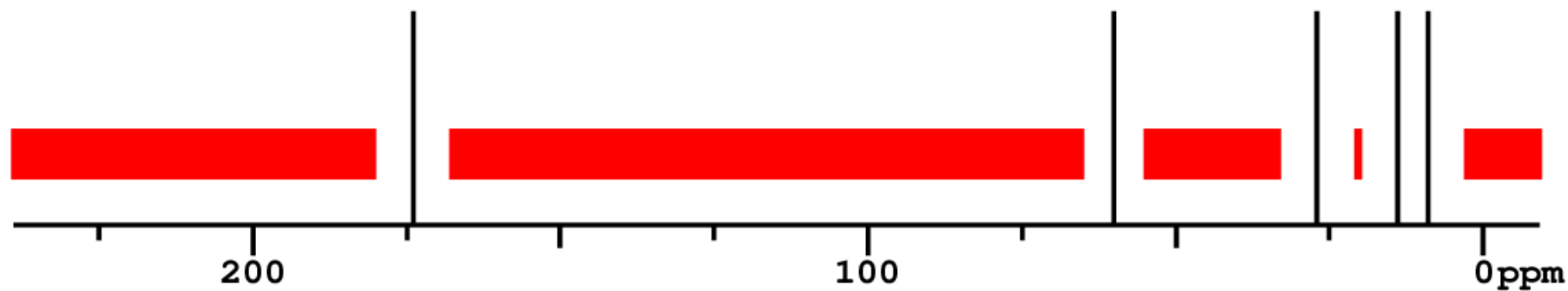
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

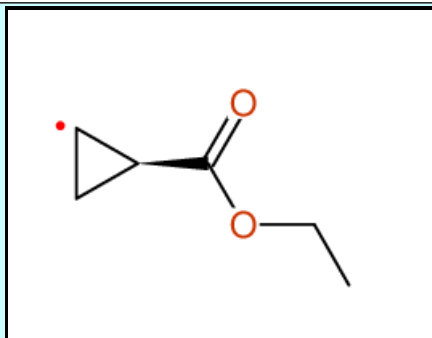
No line in reference: [red bar]



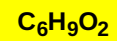
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Structure Proposal #13

Structure	Similarity Measure



Deviation = 3.30 ppm
Similarity = 100 %



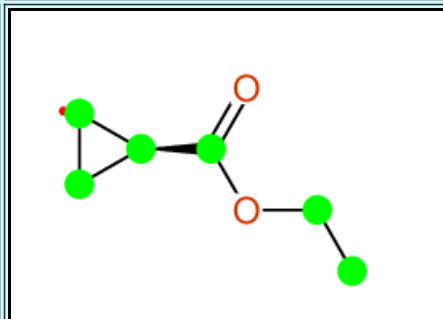
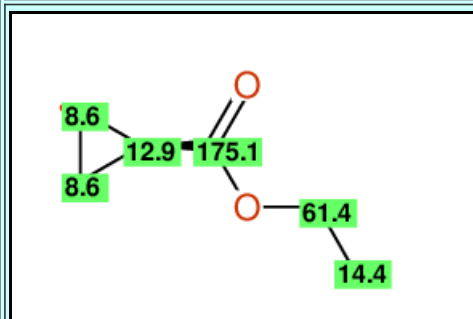
MWT = 113.07

Search Web for this structure:

[XJFUMKLBHKVVOM](#)

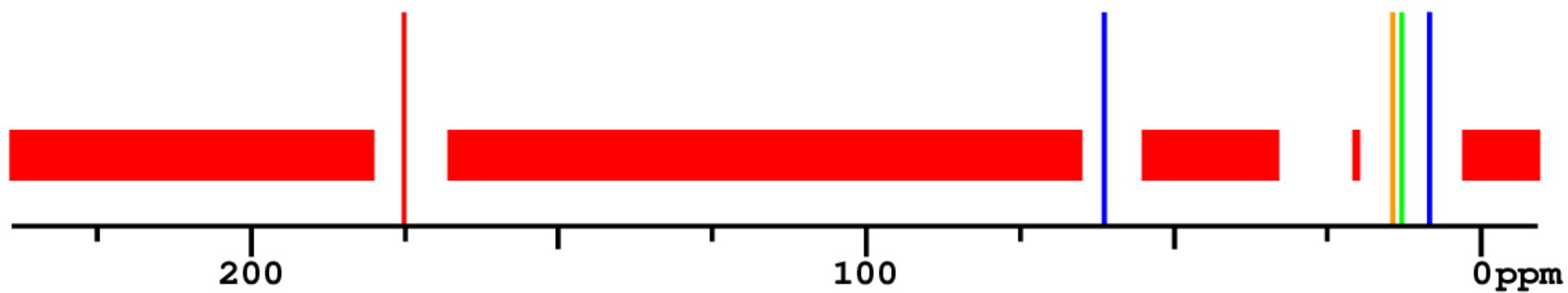
Predicted Chemical Shiftvalues

Matching Map



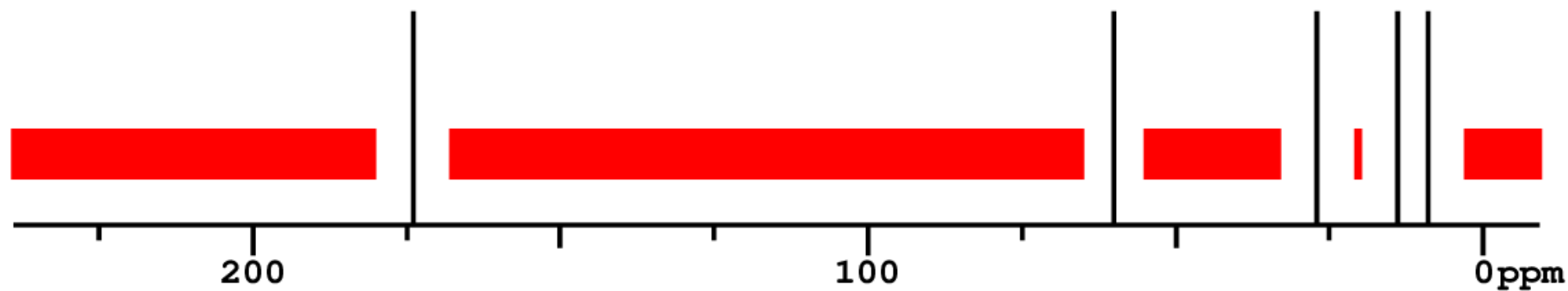
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

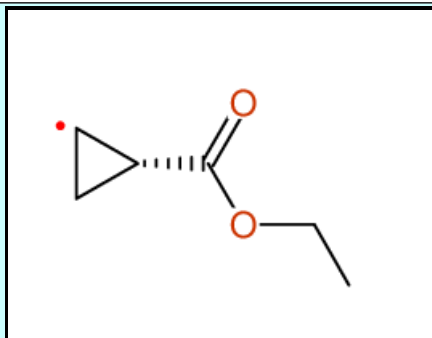
No line in reference: [red bar]



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Structure Proposal #14

Structure	Similarity Measure



Deviation = 3.30 ppm
Similarity = 100 %

$C_6H_9O_2$

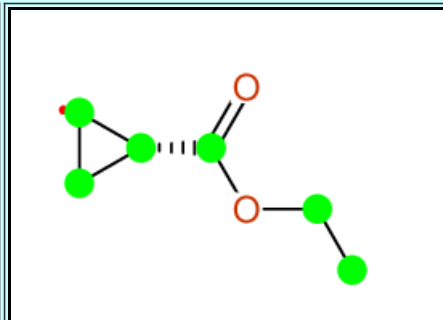
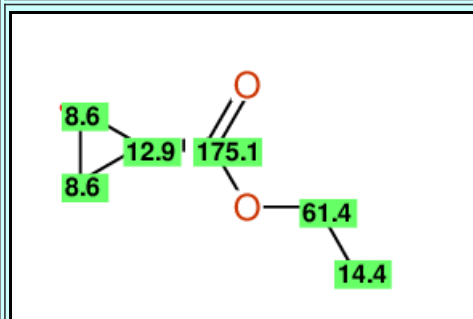
MWT = 113.07

Search Web for this structure:

[XJFUMKLBHKVVOM](#)

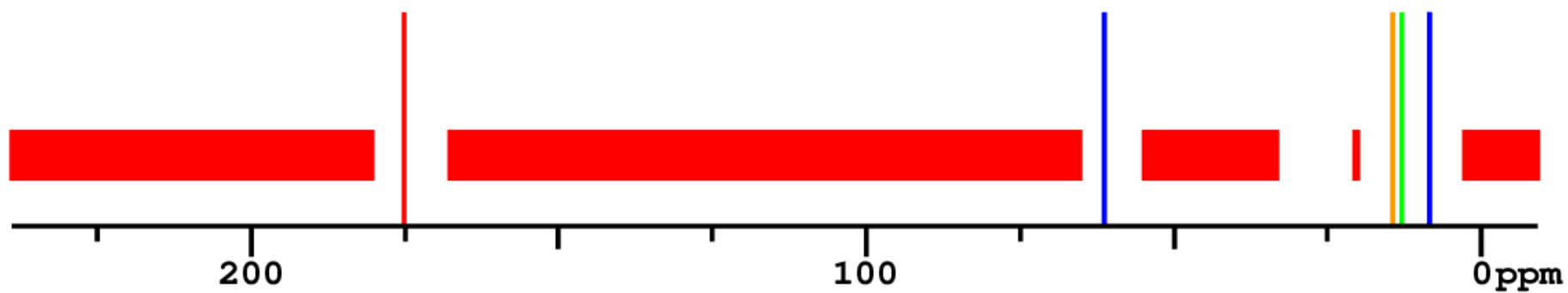
Predicted Chemical Shiftvalues

Matching Map



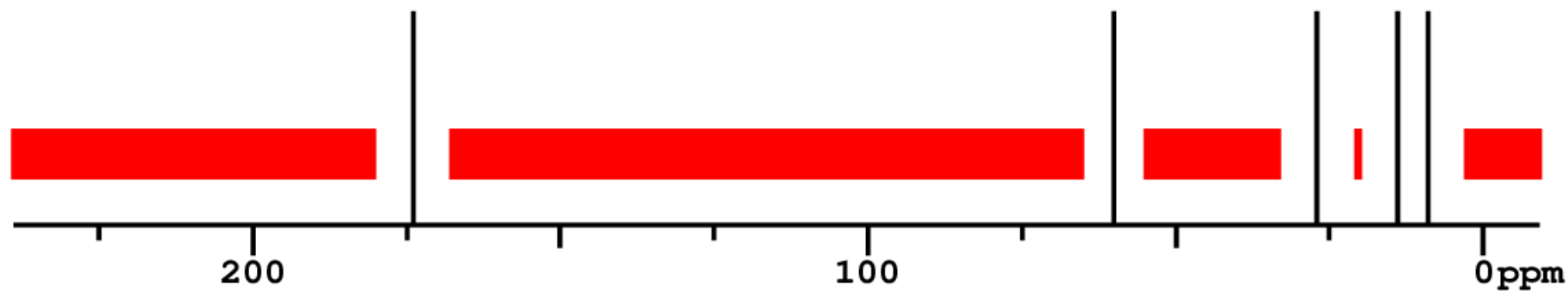
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

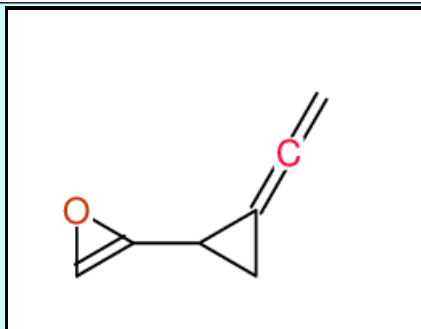
No line in reference: [red bar]



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Structure Proposal #15

Structure	Similarity Measure



Deviation = 3.63 ppm
Similarity = 100 %

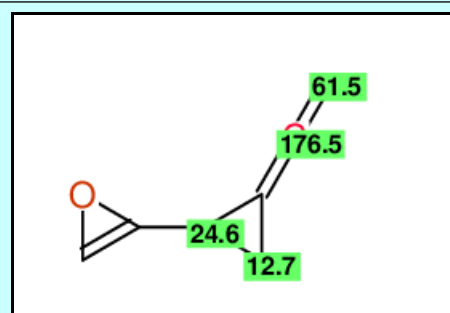
C_7H_6O

MWT = 106.08

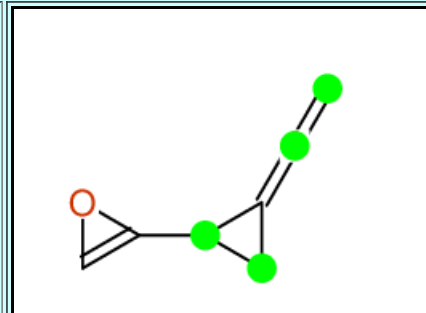
Search Web for this structure:

[SIOSIFTVQXCKHE](#)

Predicted Chemical
Shiftvalues

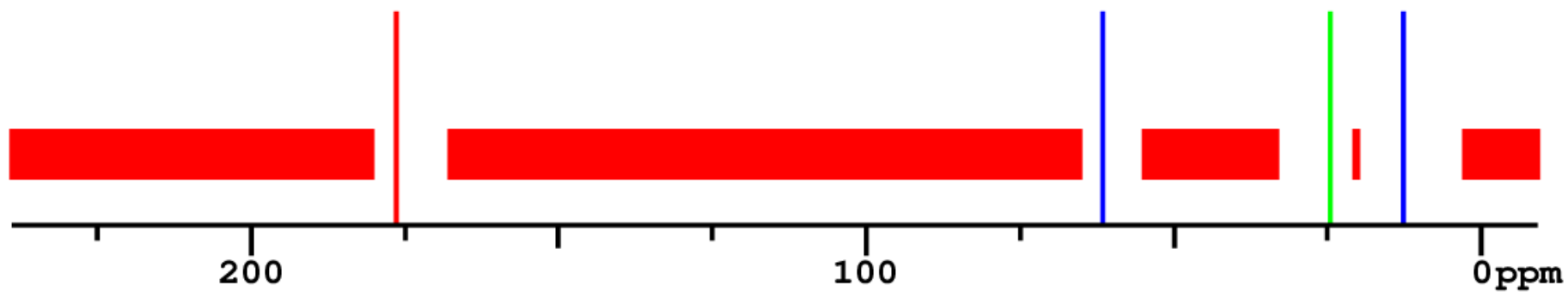


Matching Map



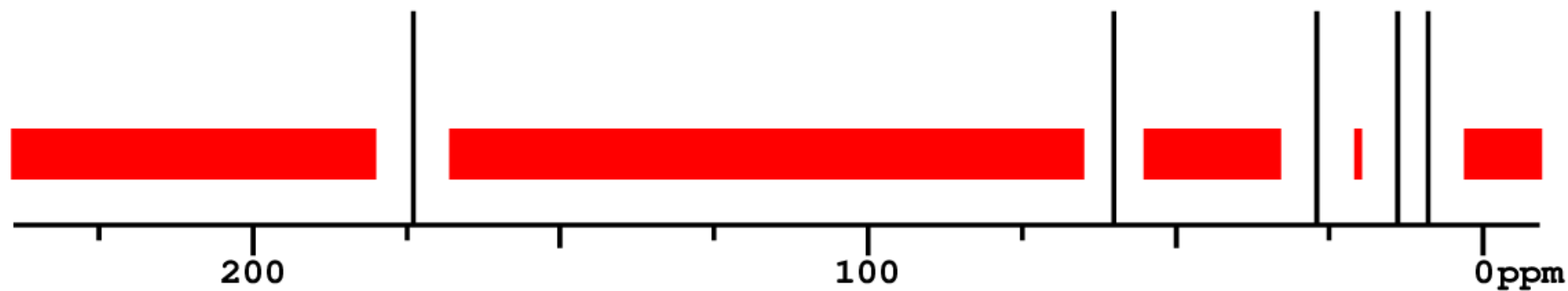
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

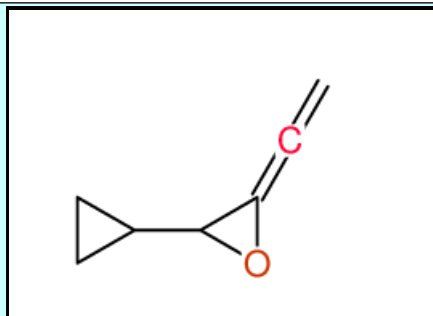
No line in reference: [red bar]



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Structure Proposal #16

Structure	Similarity Measure



Deviation = 3.98 ppm
Similarity = 100 %

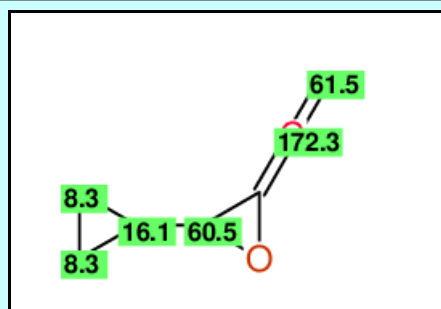
C_7H_8O

MWT = 108.08

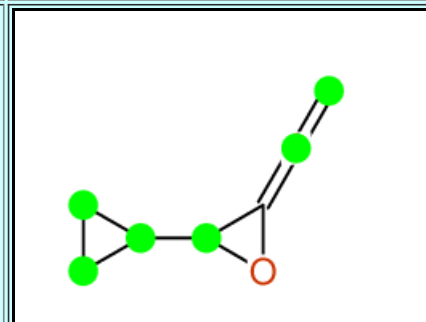
Search Web for this structure:

[SQWBZVNZMXUDFY](#)

Predicted Chemical
Shiftvalues

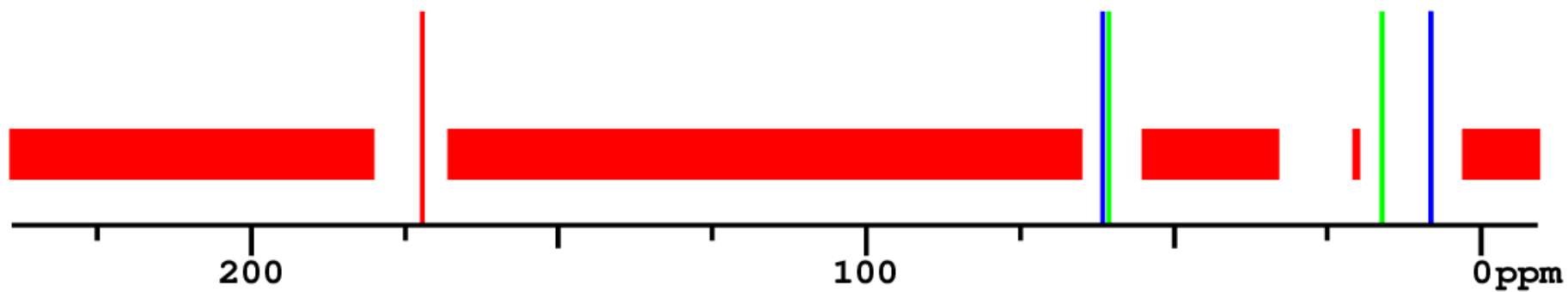


Matching Map



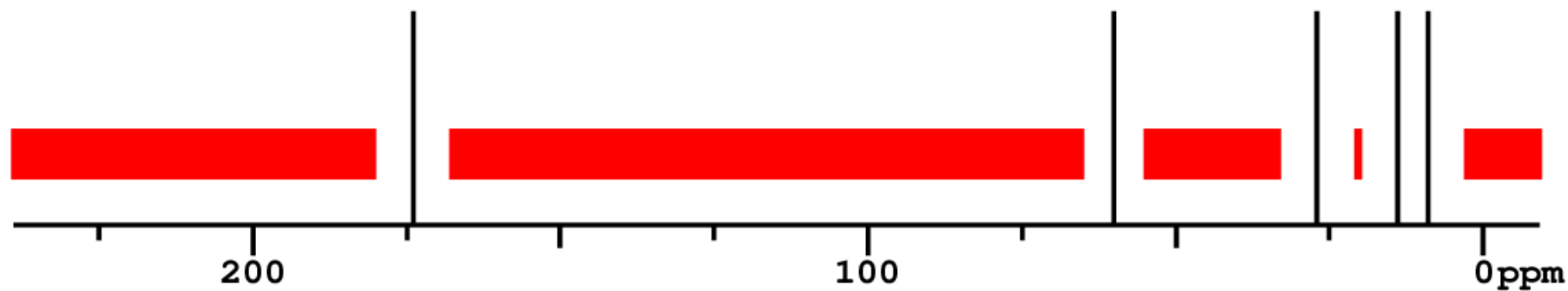
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

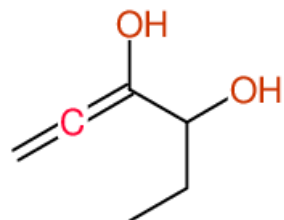
No line in reference: [red bar]



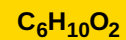
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Structure Proposal #17

Structure	Similarity Measure



Deviation = 4.72 ppm
Similarity = 80 %
(Different pattern)



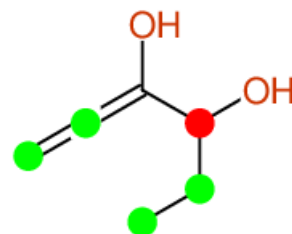
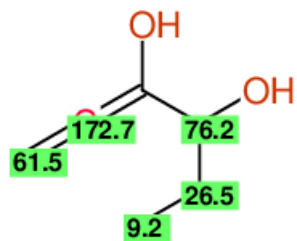
MWT = 114.07

Search Web for this structure:

[BIFODGMOCCJWOI](#)

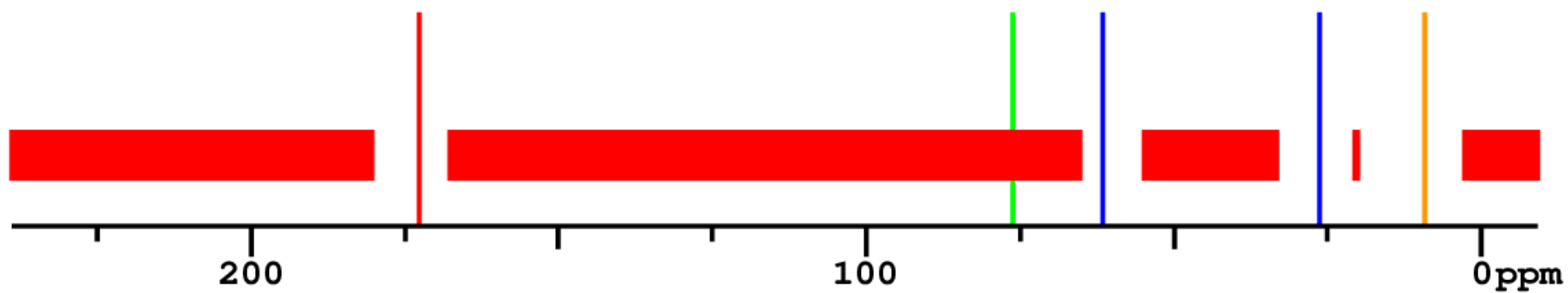
Predicted Chemical
Shiftvalues

Matching Map



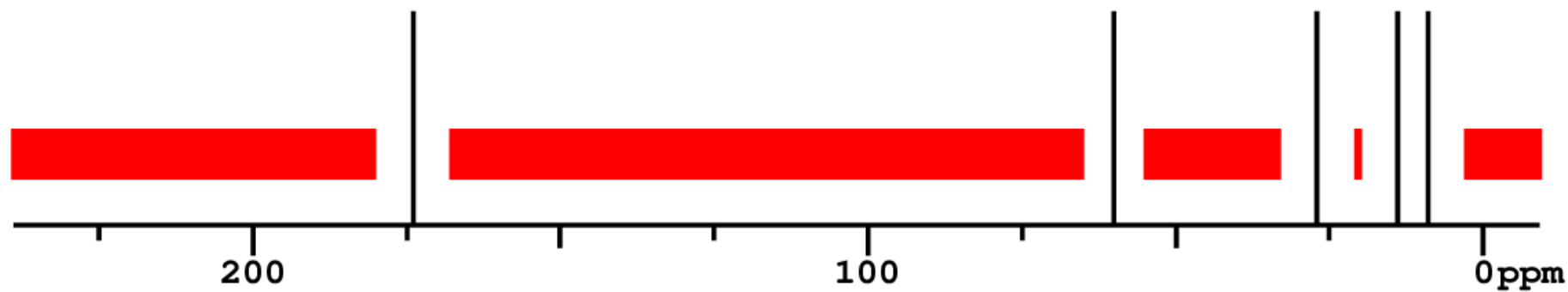
Predicted shift values

Signal multiplicity: S D T Q O E P ?



Experimental shift values

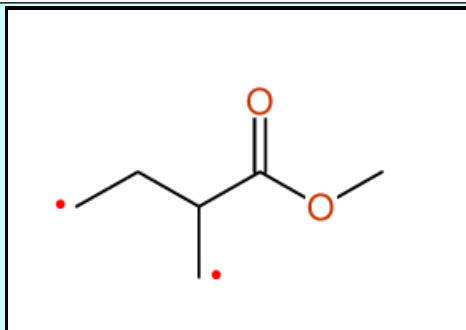
No line in reference: [red bar]



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Structure Proposal #18

Structure	Similarity Measure



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



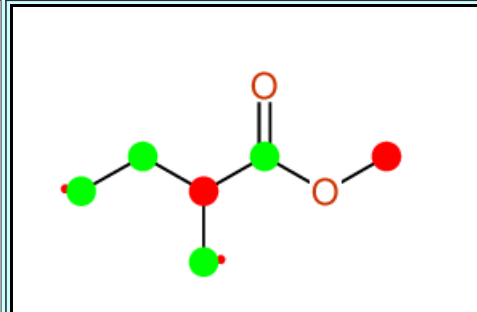
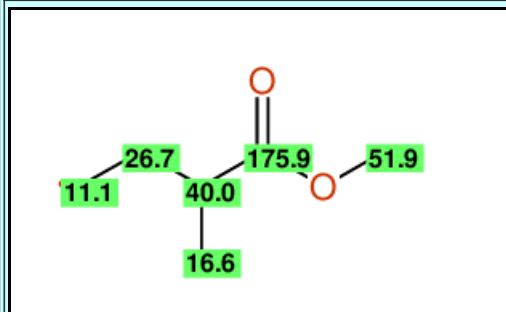
MWT = 114.07

Search Web for this structure:

[YTEGYFGYGIPBK](#)

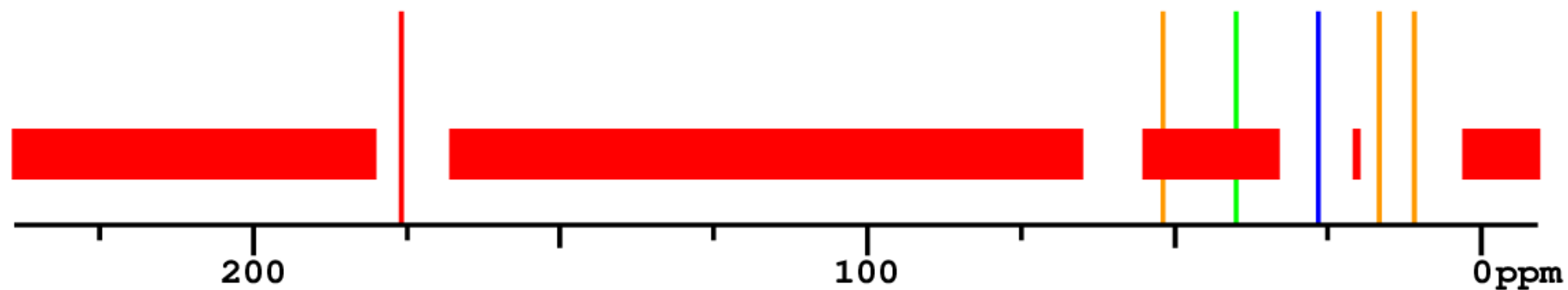
Predicted Chemical Shiftvalues

Matching Map




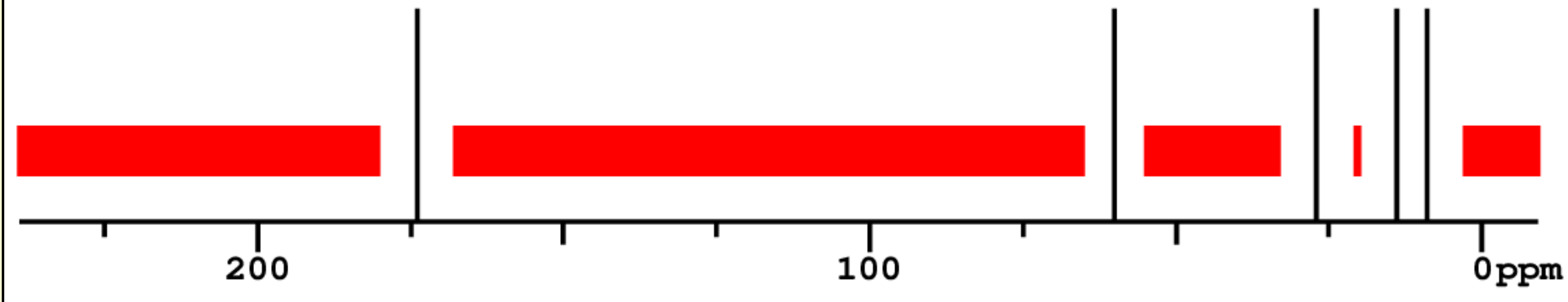
Predicted shift values

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



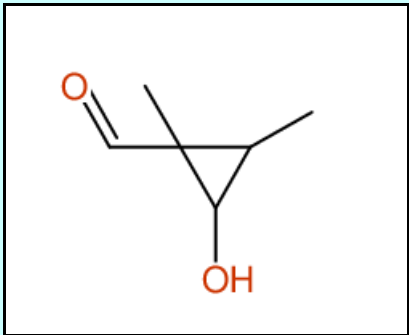
Experimental shift values

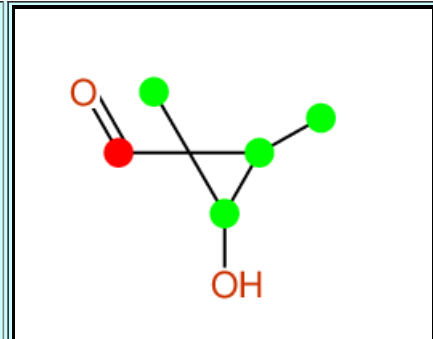
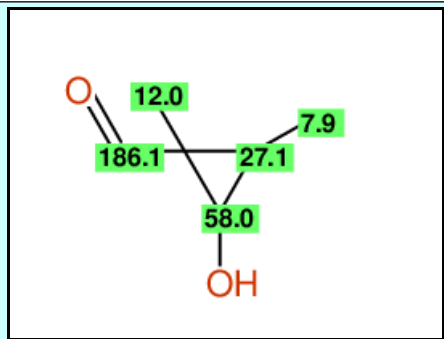
No line in reference: 



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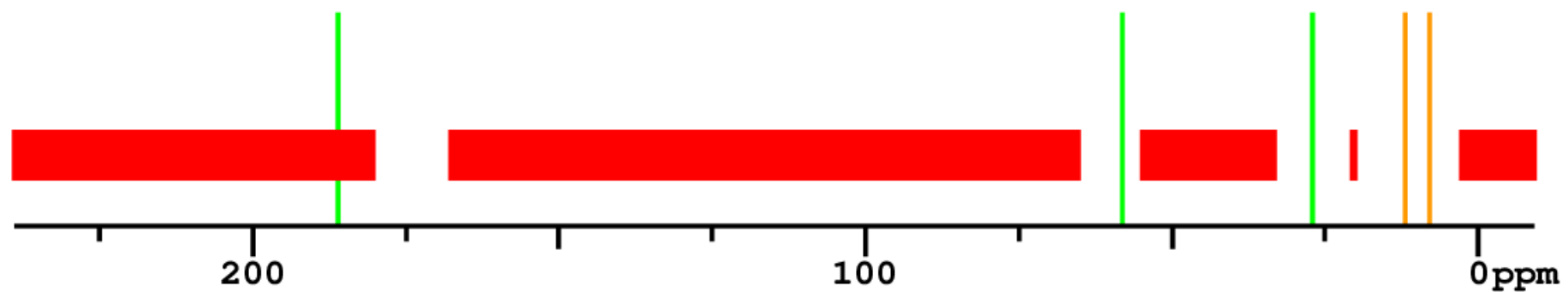
Structure Proposal #19

Structure	Similarity Measure
	<p>Deviation = 5.61 ppm Similarity = 80 % (Different pattern)</p> <p>$C_6H_{10}O_2$</p> <p>MWT = 114.07</p> <p>Search Web for this structure: HIHLRSKFLUZMEZ</p>
Predicted Chemical Shiftvalues	Matching Map



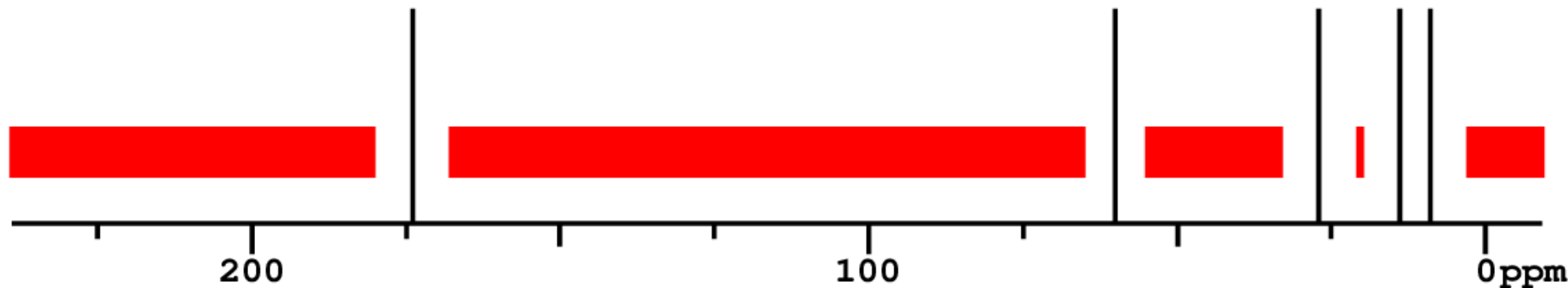
Predicted shift values

Signal multiplicity: S D T Q O E P ?



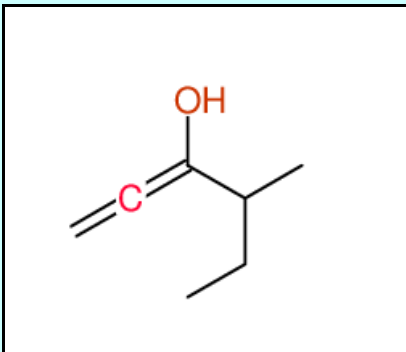
Experimental shift values

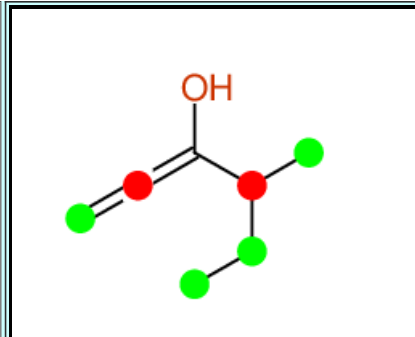
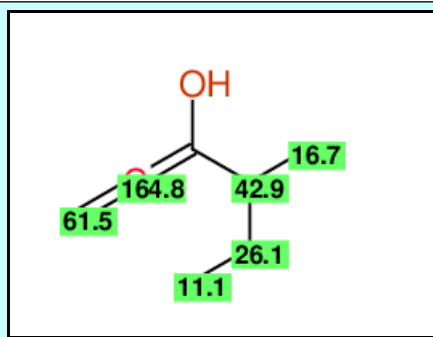
No line in reference: 



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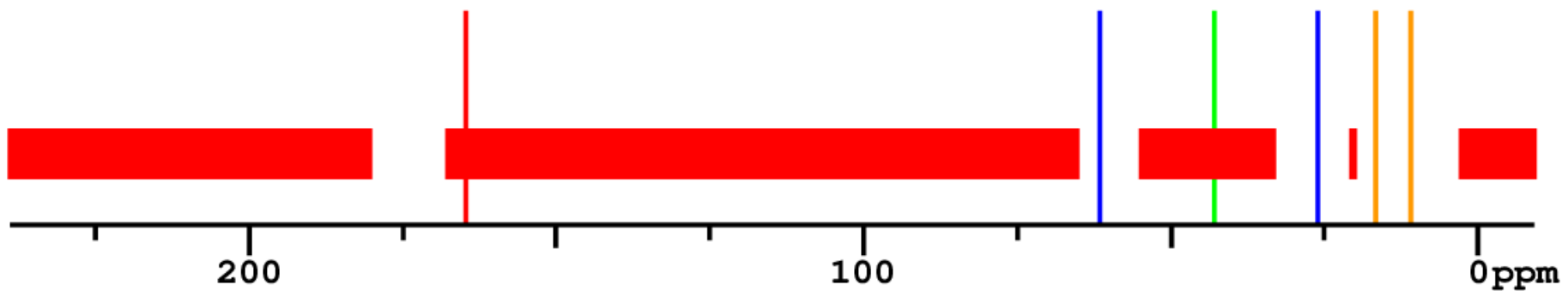
Structure Proposal #20

Structure	Similarity Measure
	<p>Deviation = 6.01 ppm Similarity = 67 % (Different pattern)</p> <p>$C_7H_{12}O$</p> <p>MWT = 112.08</p> <p>Search Web for this structure: VNLWRJLKFZXXCL</p>
Predicted Chemical Shiftvalues	Matching Map



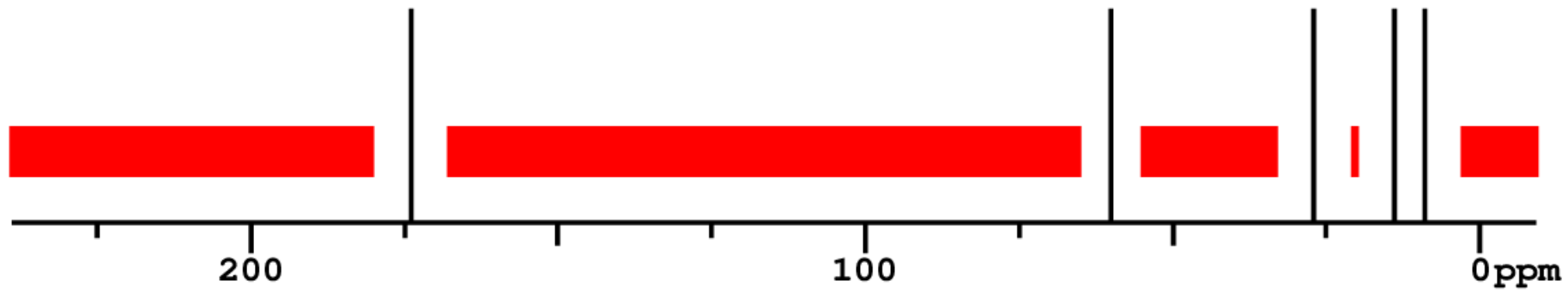
Predicted shift values

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



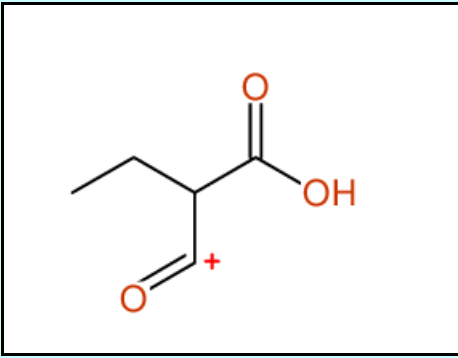
Experimental shift values

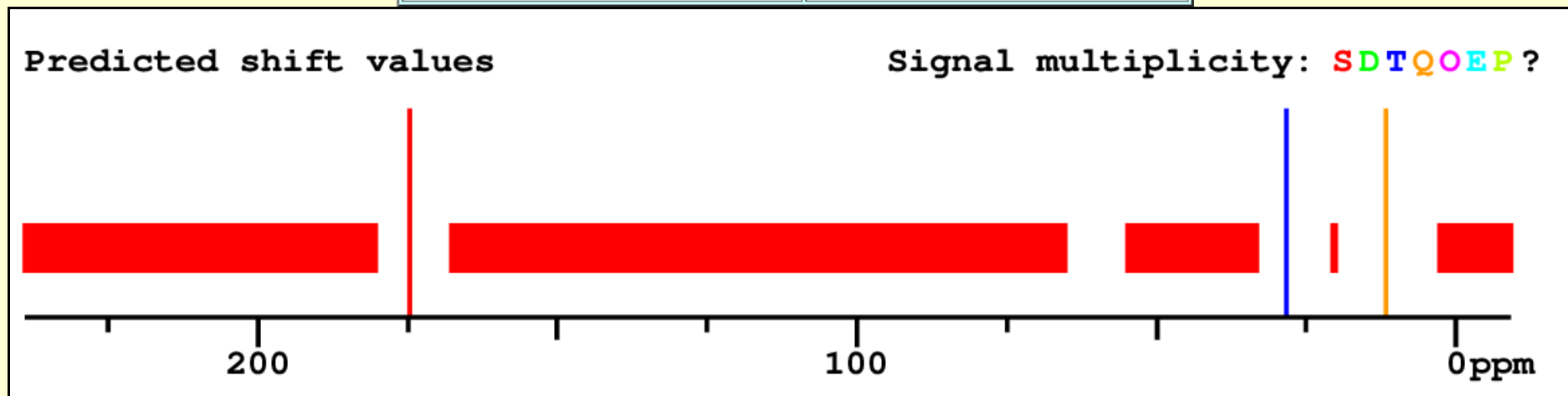
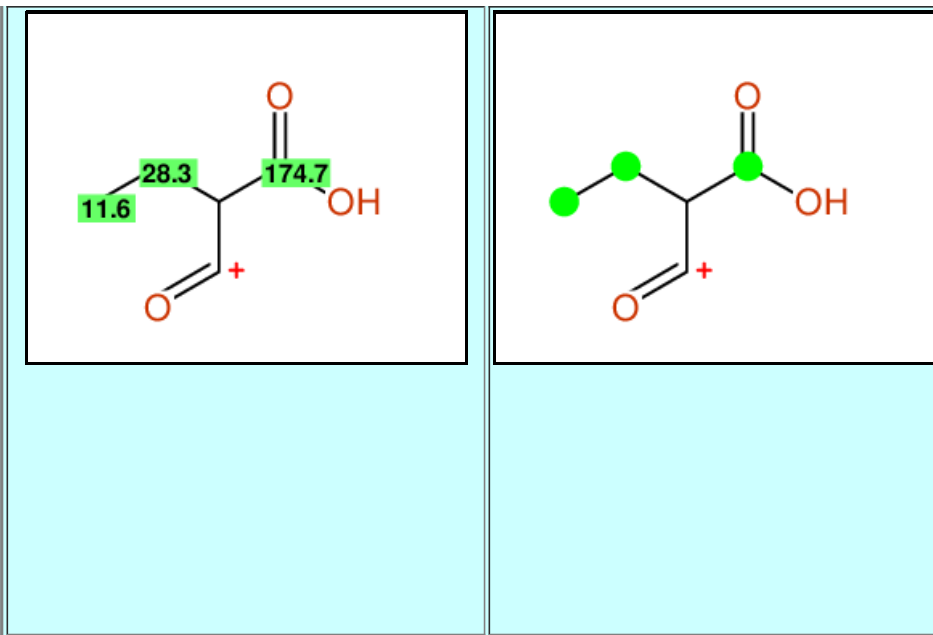
No line in reference: 




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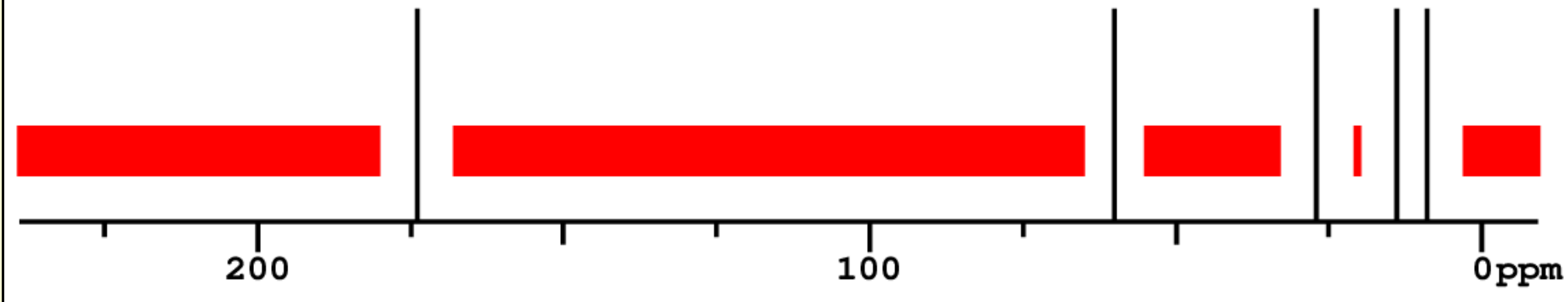
Structure Proposal #21

Structure	Similarity Measure
	Deviation = 8.84 ppm Similarity = 100 % C ₅ H ₆ O ₃ MWT = 114.06 Search Web for this structure: XKQXOPMMXGTEQA
Predicted Chemical Shiftvalues	Matching Map



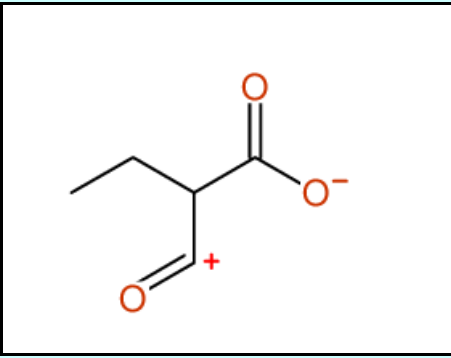
Experimental shift values

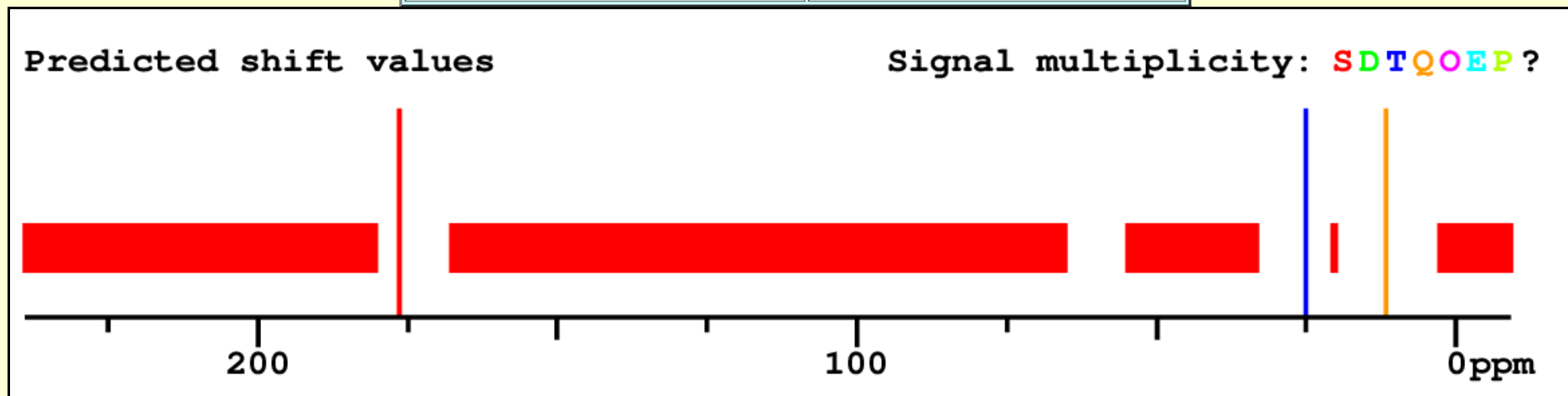
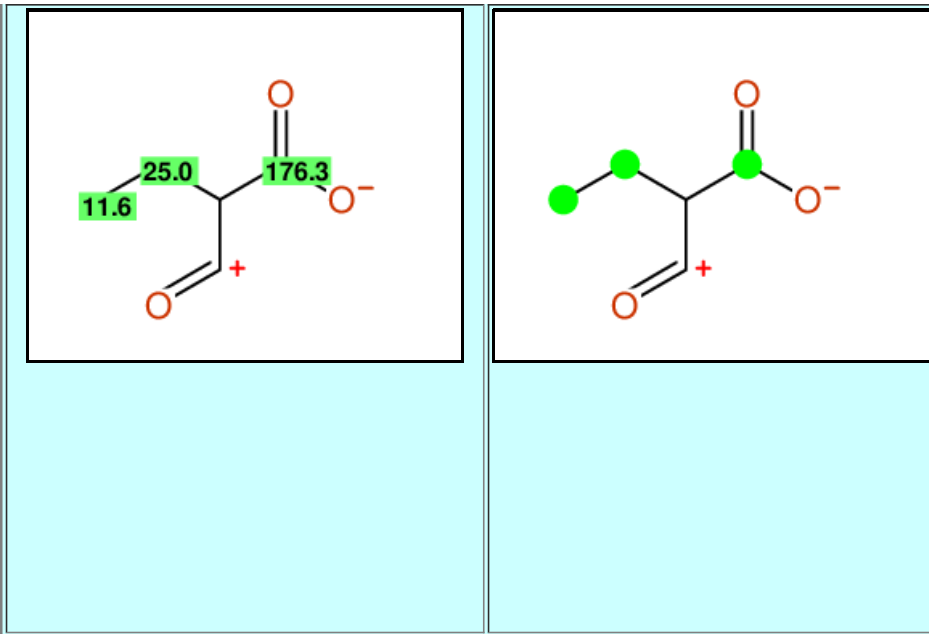
No line in reference: 



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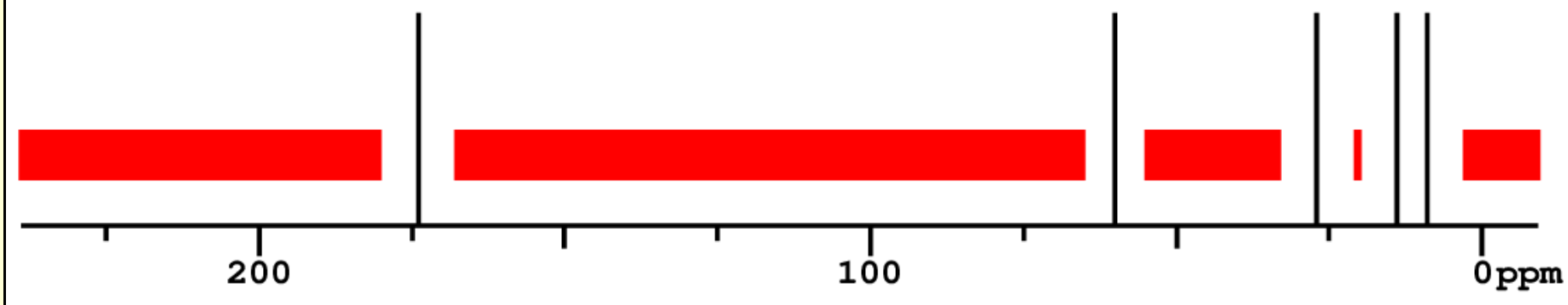
Structure Proposal #22

Structure	Similarity Measure
	Deviation = 9.70 ppm Similarity = 100 % C ₅ H ₆ O ₃ MWT = 114.06 Search Web for this structure: XKQXOPMMXGTEQA
Predicted Chemical Shiftvalues	Matching Map



Experimental shift values

No line in reference: 

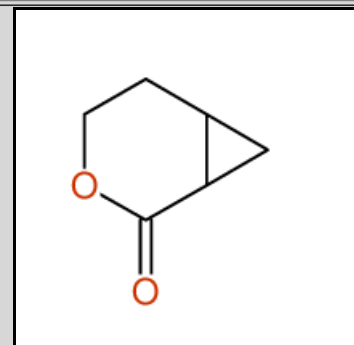


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Summary of the 2 most frequently occurring parent ring systems
within the 9 best-fitting entries

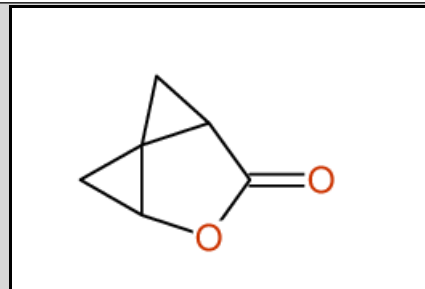
Occurrence:

1 in 9



Occurrence:

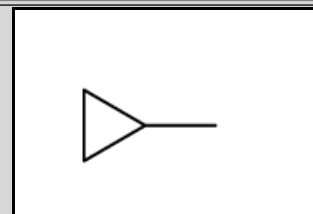
1 in 9



**Summary of the 6 most frequently occurring parent ring systems
within the 19 best-fitting entries**

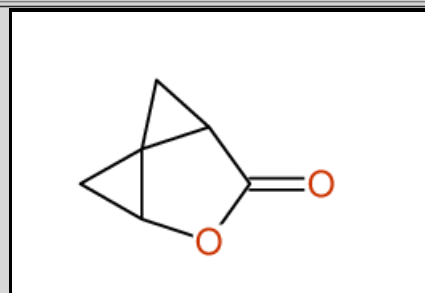
Occurrence:

4 in 19



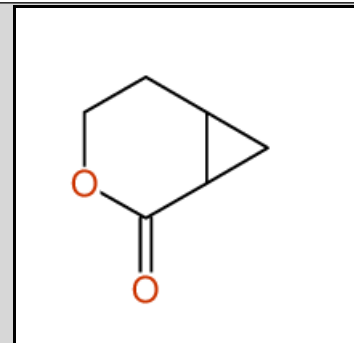
Occurrence:

1 in 19



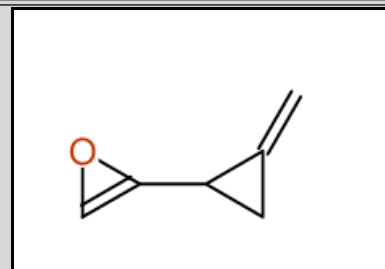
Occurrence:

1 in 19



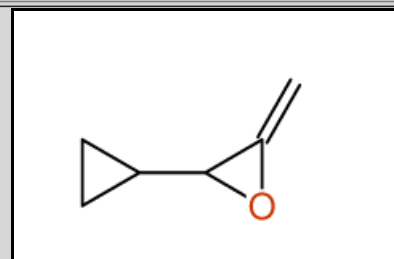
Occurrence:

1 in 19



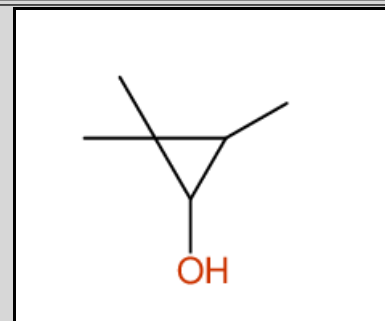
Occurrence:

1 in 19



Occurrence:

1 in 19



Summary of Processing

Checking existence of data and counting them:	177,099,966 entries in 3.226 seconds
Applying restraints from elemental composition:	8.145 seconds, 5,102,397 entries remain
Applying restraints from number of signals:	3.976 seconds, 218,318 entries remain
Searching 3,082,356,159 chemical shift values line-per-line:	44.786 seconds
Best 1,591 entries selected for analysis:	3.580 seconds
Ranking of 1,591 entries by similarity:	100.314 seconds
Deviation of best match:	0.81 ppm
Creating table and linking 1,591 structures to 475,803 INCHIKEY-pages:	1.181 seconds
Detailed Analysis of 22 structures including graphical representation:	10.633 seconds
Analysis of 19 structures for common parent ring systems:	0.003 seconds
Total CPU-usage:	177.559 seconds
Data transferred from disk:	1,814 MBytes out of 2,744,055 MBytes
Program version:	20200916_2-3D-zip/00
Machine:	I9-9900K / 16x3.60GHz

**Page written by Wolfgang Robien using CSEARCH-Technology
Page written on 2021:05:19 at 19:09
Page finished on 2021:05:19 at 19:15**

Have a nice day !