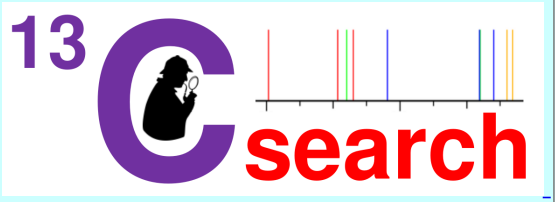
Spectral Similarity Search based on 74,435,185 Structures from PUBCHEM using CSEARCH - Technology

Description of Request

Please cite this service as:

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

Request submitted via:	
Requested by:	**test@test123.abc.info**
Requested on:	**2021:05:19 at 19:07**

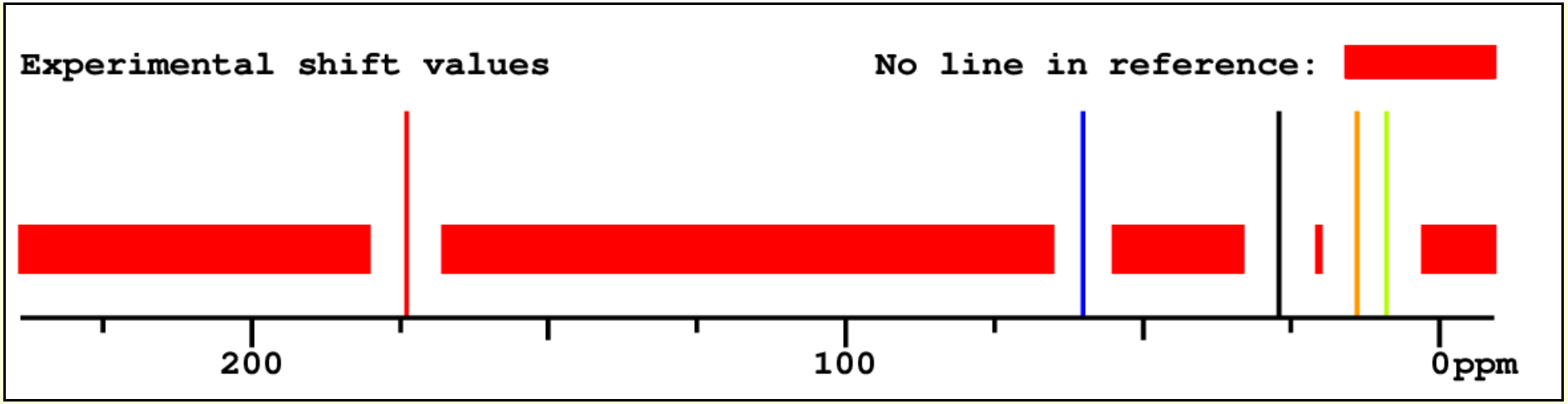
This page will be kept for 30 days here

Name of Project:	**Test1**

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

Summary of Supplied Data

Peaklist given - consists of 5 Lines				
Line number	**Chemical Shift (ppm)**	**Multiplicity**	**Hydrogens**	**Deviation (ppm)**
1	**174.00**	**S**	**C**	**3.00**
2	**60.00**	**T**	**CH_2**	**2.50**
3	**27.00**	**?**	**C or CH or CH_2 or CH_3**	**3.00**
4	**14.00**	**Q**	**CH_3**	**3.00**
5	**9.00**	**P**	**CH or CH_2 or CH_3**	**3.00**



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

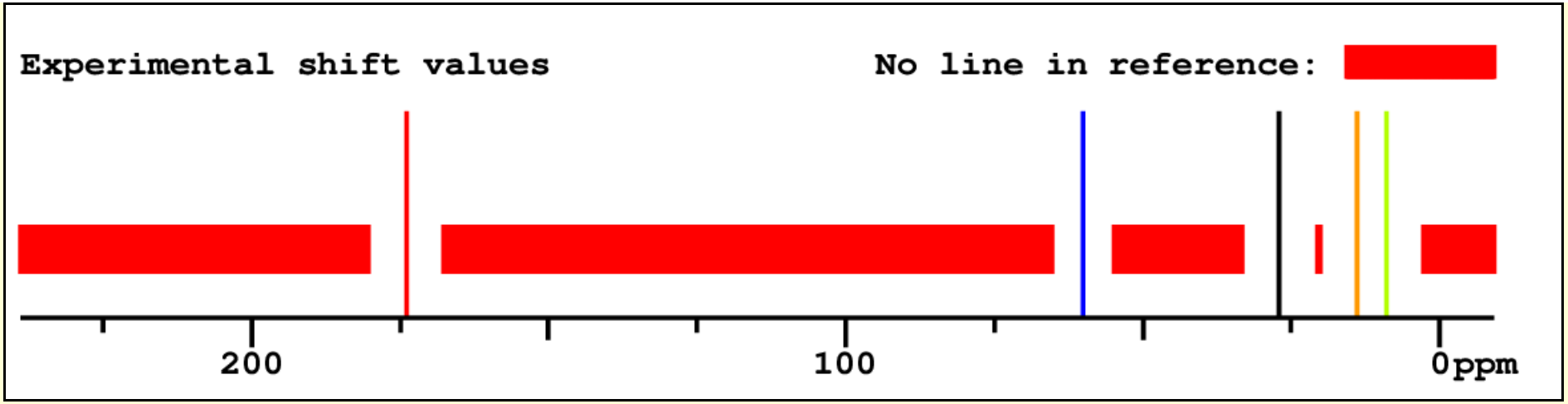
P	Element must be absent
S	Element must be absent
F	Element must be absent
Cl	Element must be absent
Br	Element must be absent
I	Element must be absent
other	Element must be absent

Elemental Composition of Reference Structures	
Total number of reference compounds:	74,435,185
Compounds containing: N	67,903,871
Compounds containing: O	67,577,895
Compounds containing: P	930,048
Compounds containing: S	23,841,191
Compounds containing: F	13,496,062
Compounds containing: Cl	13,294,181
Compounds containing: Br	4,754,113
Compounds containing: I	705,469
Compounds containing: other	1,987,940

Available entries at each Screening-Step	
Total number of entries:	74,435,185

Applying requested elemental composition:	2,773,229 entries remain
Applying requested number of signals:	170,467 entries remain

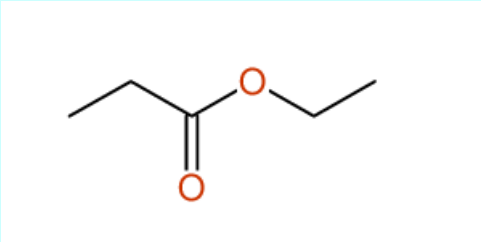
Entries per line found out of 170,467 compounds					
Line number	Chemical Shift (ppm)	Multiplicity	Deviation (ppm)	Entries found	Evaluation result
1	174.00	S	3.00	29,767	Unspecific line
2	60.00	T	2.50	22,471	Unspecific line
3	27.00	?	3.00	66,806	Unspecific line
4	14.00	Q	3.00	35,543	Unspecific line
5	9.00	P	3.00	21,626	Unspecific line



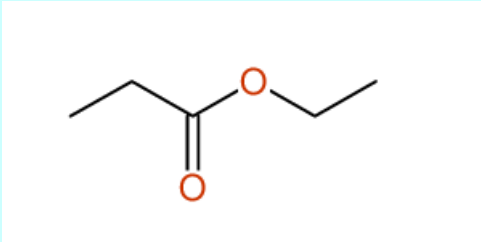
Number of coincident lines versus number of entries		
Number of coincident lines 5 Lines given	**Number of entries**	**Further Processing**
5	**129**	**Selected for detailled analysis**
4	**1,433**	**Selected for detailled analysis**
3	**8,837**	
2	**35,013**	
1	**73,299**	

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

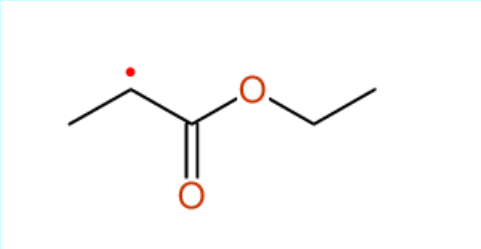
0.87 - 0.87ppm	3x found	FKRCODPIKNYEAC



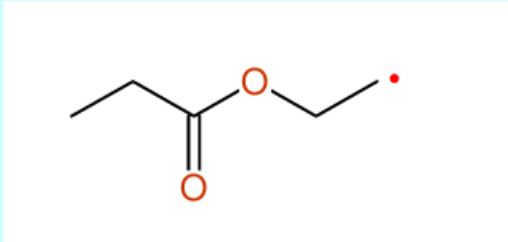
0.87 - 0.87ppm	1x found	BYLOWVUCDFUYIQ



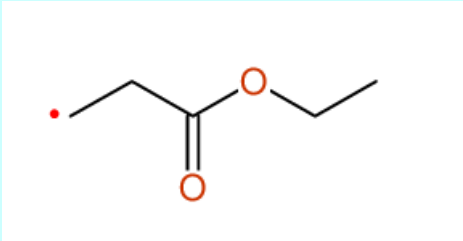
0.87 - 0.87ppm	1x found	UPRLWNPAOPKPCE



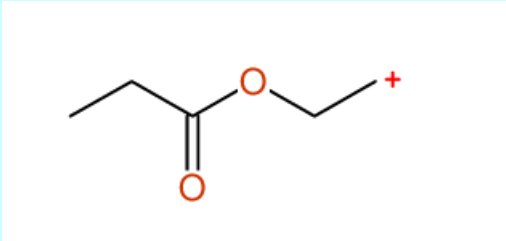
0.87 - 0.87ppm	1x found	IRGLFRDZYNBBCO



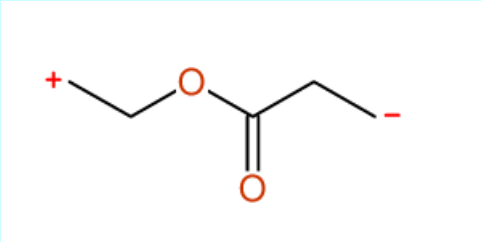
0.87 - 0.87ppm	1x found	SQKCNILPACLIRC



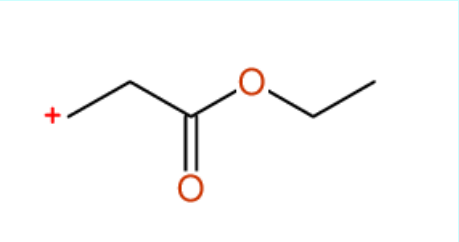
0.87 - 0.87ppm	1x found	GOKITYWXYBHPKU



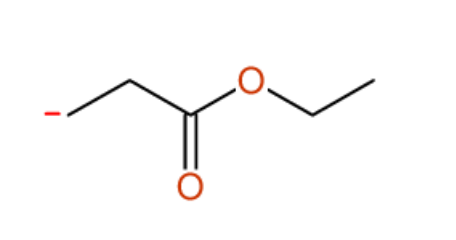
0.87 - 0.87ppm	1x found	LVCAAHDUTLIBML



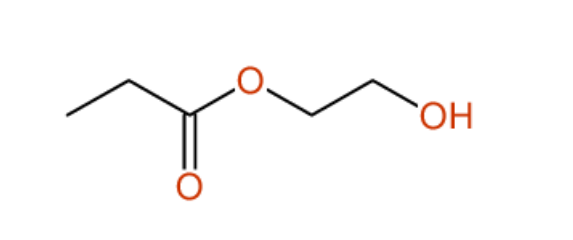
0.87 - 0.87ppm	1x found	MUQMZQYQIIZBIT



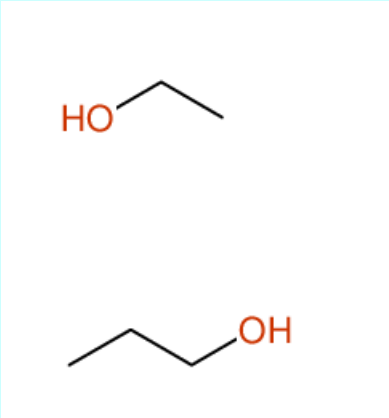
0.87 - 0.87ppm	1x found	NWIUUTFORIXPJC



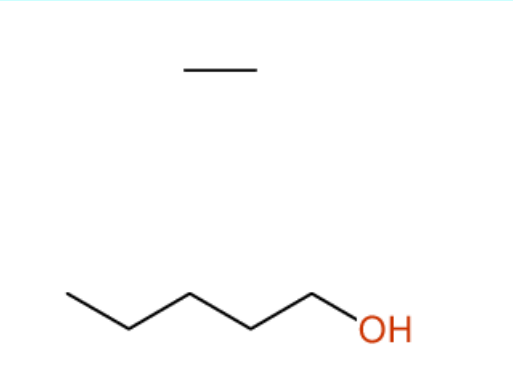
2.02 - 2.02ppm	1x found	SFAMKDPMPDEXGH



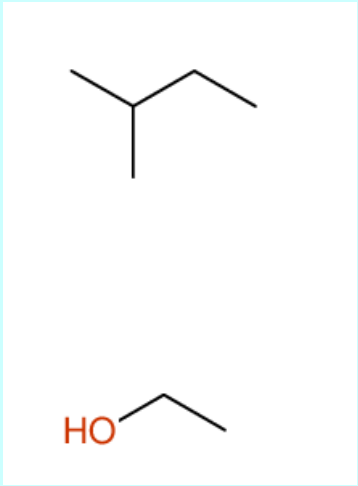
2.62 - 2.62ppm	1x found	OMRDZQXXMYCHBU



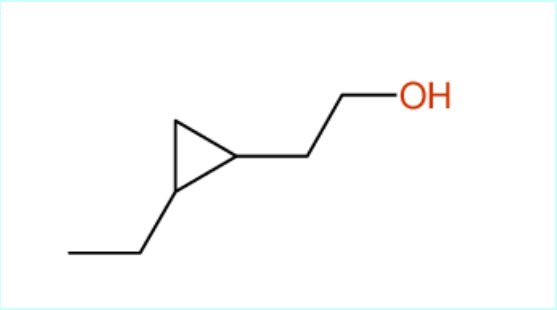
2.98 - 2.98ppm	1x found	ZARMDFHSJSIZKQ



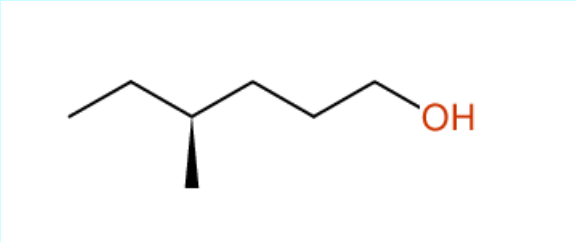
3.16 - 3.16ppm	1x found	FOXQTCHXXJKLNK



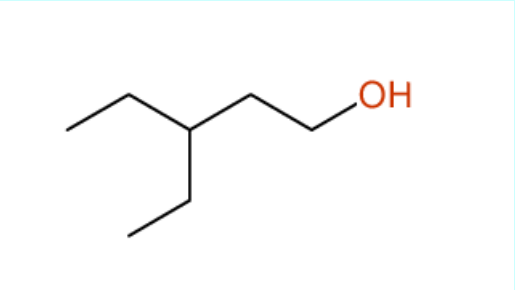
3.49 - 3.49ppm	1x found	IPKMDCPNAOYUEB



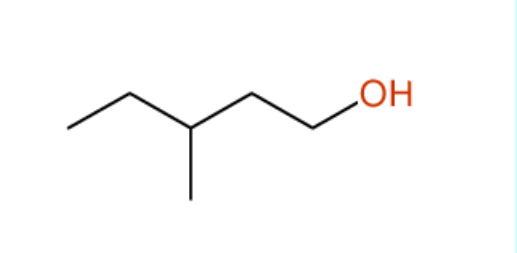
4.01 - 4.01ppm	3x found	YNPVNLWKVZZBTM



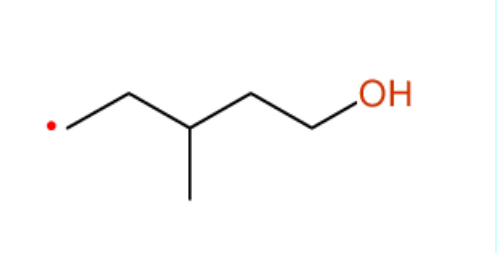
4.36 - 4.36ppm	1x found	DVEFUHVVWJONKR



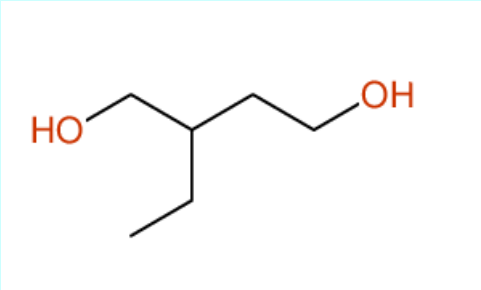
4.64 - 4.64ppm	3x found	IWTBVKIGCDZRPL



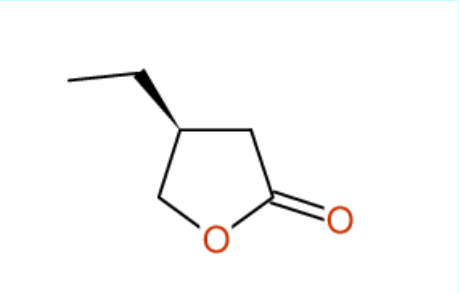
4.64 - 4.64ppm	1x found	FCACGIMTGMLTKJ



4.98 - 4.98ppm	3x found	CYVMBANVYOZFIG



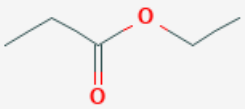
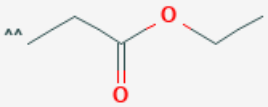
6.77 - 6.88ppm	2x found	MDQZVJSUBKPTHG

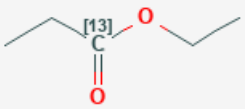
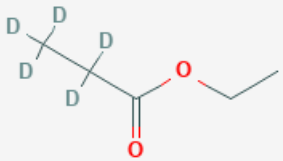


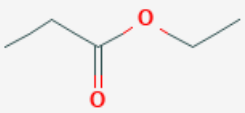
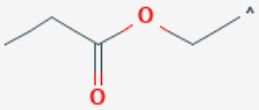
1,562 Structure proposals found for your C-NMR Spectrum

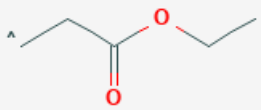
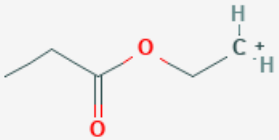
50 Entries will be shown because of your selection of additional constraints

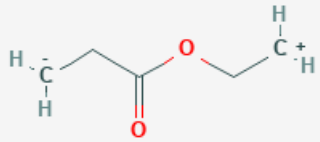
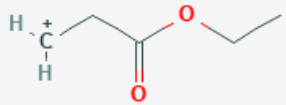
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼

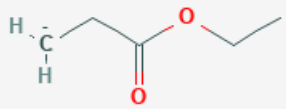
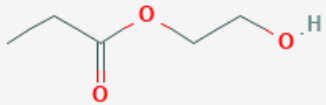
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_{10}O_2$ MWT = 102.055	Proposal #1 FKRCODPIKNYEAC-UHFFFAOYSA-N PUBCHEM Compound: 7749	Availability of NMR-Data in CSEARCH
0.87 Details		$C_5H_8O_2$ MWT = 100.055	Proposal #2 BYLOWVUCDFUYIQ-UHFFFAOYSA-N PUBCHEM Compound: 45120489	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_{10}O_2$ MWT = 103.055	Proposal #3 FKRCODPIKNYEAC-HOSYLAQJSA-N PUBCHEM Compound: 12229103	Availability of NMR-Data in CSEARCH
0.87 Details		$C_5H_{10}O_2$ MWT = 107.055	Proposal #4 FKRCODPIKNYEAC-WNWXXORZSA-N PUBCHEM Compound: 89254459	Availability of NMR-Data in CSEARCH

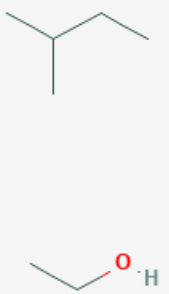
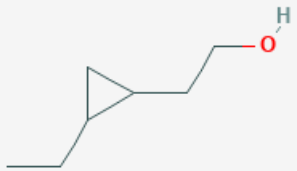
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_9O_2$ MWT = 101.055	Proposal #5 UPRLWNPAOPKPCE-UHFFFAOYSA-N PUBCHEM Compound: 5371171	
0.87 Details		$C_5H_9O_2$ MWT = 101.055	Proposal #6 IRGLFRDZYNBBCO-UHFFFAOYSA-N PUBCHEM Compound: 57419189	

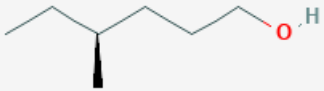
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_9O_2$ MWT = 101.055	Proposal #7 SQKCNILPACLIRC-UHFFFAOYSA-N PUBCHEM Compound: 12568583	
0.87 Details		$C_5H_9O_2^+$ MWT = 101.055	Proposal #8 GOKITYWXYBHPKU-UHFFFAOYSA-N PUBCHEM Compound: 57582310	

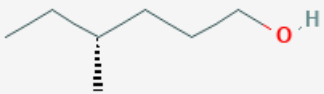
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_8O_2$ MWT = 100.055	Proposal #9 LVCAAHDUTLIBML-UHFFFAOYSA-N PUBCHEM Compound: 53630283	
0.87 Details		$C_5H_9O_2^+$ MWT = 101.055	Proposal #10 MUQMZQYQIIZBIT-UHFFFAOYSA-N PUBCHEM Compound: 91194346	

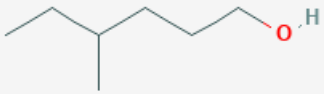
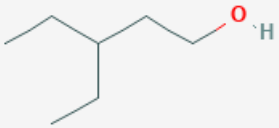
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
0.87 Details		$C_5H_9O_2^-$ MWT = 101.055	Proposal #11 NWIUUTFORIXPJC-UHFFFAOYSA-N PUBCHEM Compound: 91508541	
2.02 Details		$C_5H_{10}O_3$ MWT = 118.055	Proposal #12 SFAMKDPMPDEXGH-UHFFFAOYSA-N PUBCHEM Compound: 545098	

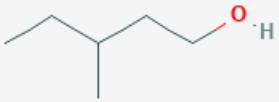
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
2.62 Details	 	$C_5H_{14}O_2$ MWT = 106.055	Proposal #13 OMRDZQXXMYCHBU-UHFFFAOYSA-N PUBCHEM Compound: 9793718	
2.98 Details	 	$C_7H_{18}O$ MWT = 118.077	Proposal #14 ZARMDFHSJSIZKQ-UHFFFAOYSA-N PUBCHEM Compound: 54537300	

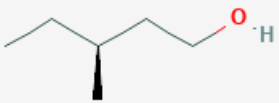
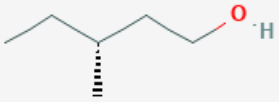
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
3.16 Details		$C_7H_{18}O$ MWT = 118.077	Proposal #15 FOXQTCHXXJKLNK-UHFFFAOYSA-N PUBCHEM Compound: 21646453	
3.49 Details Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #16 IPKMDCPNAOYUEB-UHFFFAOYSA-N PUBCHEM Compound: 23329956	Availability of NMR-Data in CSEARCH

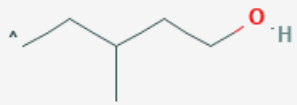
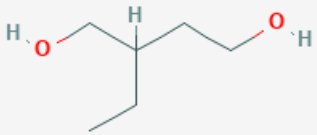
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.01 Details Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #17 YNPVNLWKVZZBTM-ZETCQYMHSA-N PUBCHEM Compound: 13463446	Availability of NMR-Data in CSEARCH

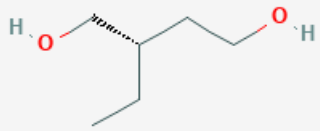
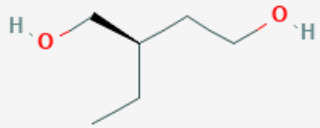
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.01 Details Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #18 YNPVNLWKVZZBTM-SSDOTTSWSA-N PUBCHEM Compound: 13463447	Availability of NMR-Data in CSEARCH

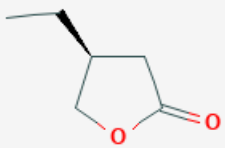
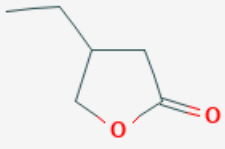
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.01 Details Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #19 YNPVNLWKVZZBTM-UHFFFAOYSA-N PUBCHEM Compound: 98346	Availability of NMR-Data in CSEARCH
4.36 Details Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #20 DVEFUHVVWJONKR-UHFFFAOYSA-N PUBCHEM Compound: 641005	Availability of NMR-Data in CSEARCH

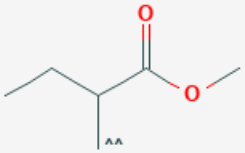
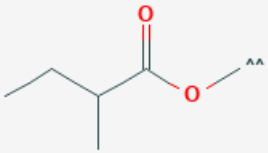
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #21 IWTBVKIGCDZRPL-UHFFFAOYSA-N PUBCHEM Compound: 11508	Availability of NMR-Data in CSEARCH

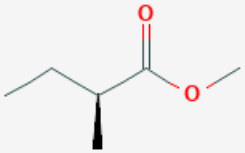
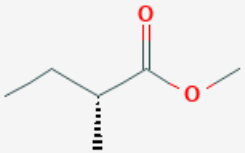
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #22 IWTBVKIGCDZRPL-LURJTMIESA-N PUBCHEM Compound: 641003	Availability of NMR-Data in CSEARCH
4.64 Details Different pattern		$C_6H_{14}O$ MWT = 102.066	Proposal #23 IWTBVKIGCDZRPL-ZCFIWIBFSA-N PUBCHEM Compound: 6999792	Availability of NMR-Data in CSEARCH

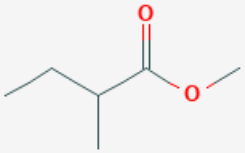
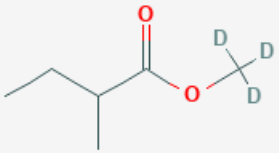
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.64 Details Different pattern		$C_6H_{13}O$ MWT = 101.066	Proposal #24 FCACGIMTGMLTKJ-UHFFFAOYSA-N PUBCHEM Compound: 57432776	
4.98 Details Different pattern		$C_6H_{14}O_2$ MWT = 118.066	Proposal #25 CYVMBANVYOZFIG-UHFFFAOYSA-N PUBCHEM Compound: 12648201	

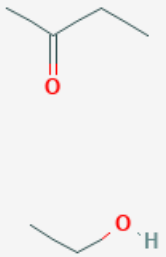
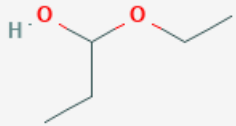
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
4.98 Details Different pattern		$C_6H_{14}O_2$ MWT = 118.066	Proposal #26 CYVMBANVYOZFIG-LURJTMIESA-N PUBCHEM Compound: 12648202	
4.98 Details Different pattern		$C_6H_{14}O_2$ MWT = 118.066	Proposal #27 CYVMBANVYOZFIG-ZCFIWIBFSA-N PUBCHEM Compound: 11804732	

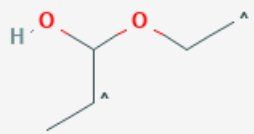
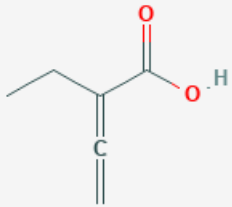
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
6.77 Details Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #28 MDQZVJSUBKPTHG-YFKPBYRVSA-N PUBCHEM Compound: 57939696	Availability of NMR-Data in CSEARCH
6.88 Details Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #29 MDQZVJSUBKPTHG-UHFFFAOYSA-N PUBCHEM Compound: 27893	Availability of NMR-Data in CSEARCH

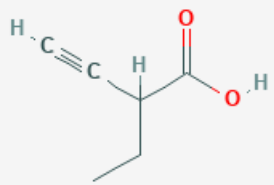
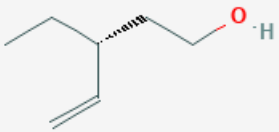
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
13.29 Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #30 YMRCZGBILKTSCL-UHFFFAOYSA-N PUBCHEM Compound: 59258212	
13.29 Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #31 OYGDMLWOJBKWLN-UHFFFAOYSA-N PUBCHEM Compound: 59990131	

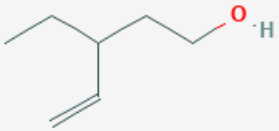
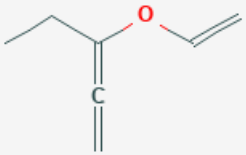
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
13.29 Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #32 OCWLYWIFNDCWRZ-YFKPBYRVSA-N PUBCHEM Compound: 643001	Availability of NMR-Data in CSEARCH
13.29 Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #33 OCWLYWIFNDCWRZ-RXMQYKEDSA-N PUBCHEM Compound: 644216	Availability of NMR-Data in CSEARCH

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
13.29 Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #34 OCWLYWIFNDCWRZ-UHFFFAOYSA-N PUBCHEM Compound: 13357	Availability of NMR-Data in CSEARCH
13.29 Different pattern		$C_6H_{12}O_2$ MWT = 119.066	Proposal #35 OCWLYWIFNDCWRZ-HPRDVNIFSA-N PUBCHEM Compound: 60069722	Availability of NMR-Data in CSEARCH

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
15.10 Different pattern		$C_6H_{14}O_2$ MWT = 118.066	Proposal #36 CASOXAYOCHCWQU-UHFFFAOYSA-N PUBCHEM Compound: 22558530	
17.85 Different pattern		$C_5H_{12}O_2$ MWT = 104.055	Proposal #37 JLBXCKSMESLGTJ-UHFFFAOYSA-N PUBCHEM Compound: 93269	Availability of NMR-Data in CSEARCH

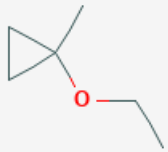
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
17.85 Different pattern		$C_5H_{10}O_2$ MWT = 102.055	Proposal #38 VOXZYDHLZQKQCB-UHFFFAOYSA-N PUBCHEM Compound: 90787265	
19.52 Different pattern		$C_6H_8O_2$ MWT = 112.066	Proposal #39 PSBUQOAVEMYGEF-UHFFFAOYSA-N PUBCHEM Compound: 15570377	

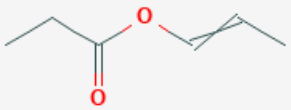
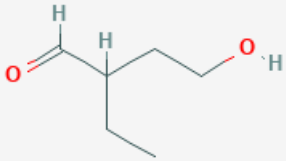
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
22.42 Different pattern		$C_6H_8O_2$ MWT = 112.066	Proposal #40 YHXLBJJLZTWBAZ-UHFFFAOYSA-N PUBCHEM Compound: 12491392	
26.40 Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #41 LRKICXFRWQUFSZ-SSDOTTSWSA-N PUBCHEM Compound: 24767552	

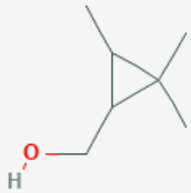
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
26.40 Different pattern		$C_7H_{14}O$ MWT = 114.077	Proposal #42 LRKICXFRWQUFSZ-UHFFFAOYSA-N PUBCHEM Compound: 86167614	
26.50 Different pattern		$C_7H_{10}O$ MWT = 110.077	Proposal #43 MFKQNKFYXTXLMB-UHFFFAOYSA-N PUBCHEM Compound: 15084427	Availability of NMR-Data in CSEARCH

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
31.36 Different pattern		$C_7H_{16}O$ MWT = 116.077	Proposal #44 KFRVYYGHSPLXSZ-UHFFFAOYSA-N PUBCHEM Compound: 13527	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
31.36 Different pattern		$C_7H_{16}O$ MWT = 119.077	Proposal #45 KFRVYYGHSPLXSZ-FIBGUPNXSA-N PUBCHEM Compound: 10534657	
31.36 Different pattern		$C_7H_{15}O$ MWT = 115.077	Proposal #46 NFHQDZUNLMHWRI-UHFFFAOYSA-N PUBCHEM Compound: 57481895	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
32.40		$C_6H_{12}O$ MWT = 100.066	Proposal #47 FSYJSAIZYZZLQM-UHFFFAOYSA-N PUBCHEM Compound: 53642689	

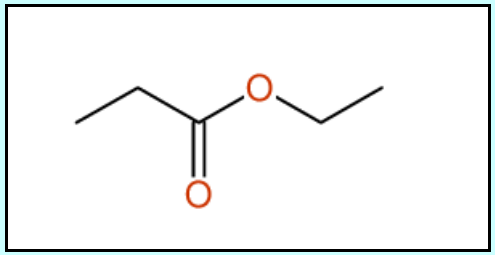
Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
35.28 Different pattern		$C_6H_{10}O_2$ MWT = 114.066	Proposal #48 AOJIRGQJECGWRU-UHFFFAOYSA-N PUBCHEM Compound: 53653613	
38.45 Different pattern		$C_6H_{12}O_2$ MWT = 116.066	Proposal #49 CBSYYWQEKMTXTJ-UHFFFAOYSA-N PUBCHEM Compound: 12367599	

Similarity (ppm) ▲▼	Structure Diagram	Molecular Formula Molecular Weight ▲▼	InChIkey	Experimental Data in CSEARCH ▲▼
38.93		$C_7H_{14}O$ MWT = 114.077	Proposal #50 SIFLEUDKOSRPAP-UHFFFAOYSA-N PUBCHEM Compound: 14202705	

Detailled Analysis

Structure Proposal #1

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_{10}O_2$

MWT = 102.06

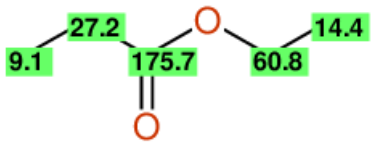
PUBCHEM

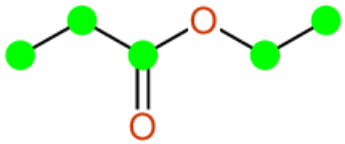
Search Web for this structure:

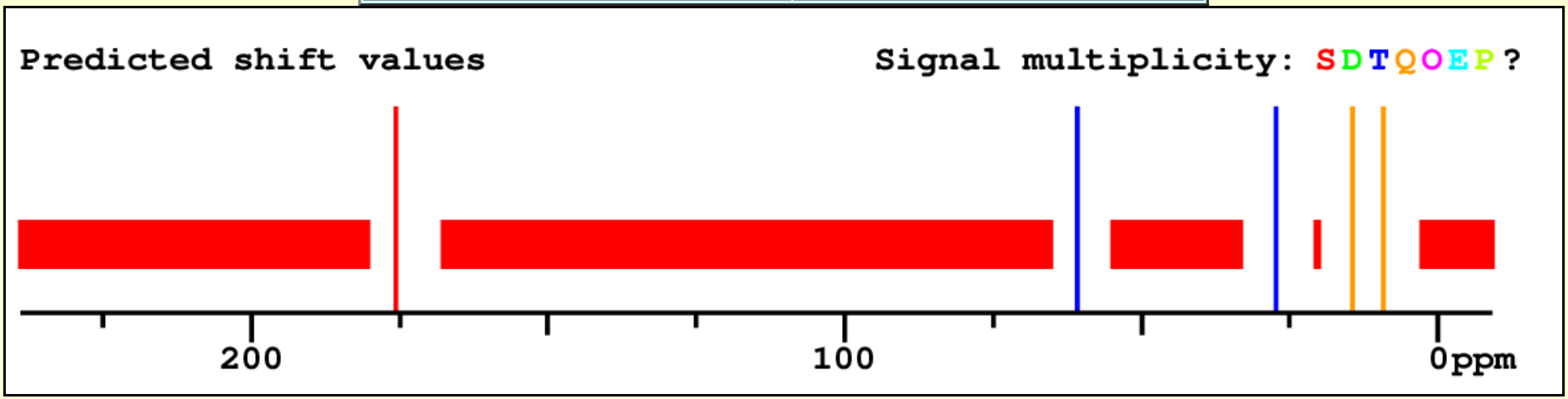
FKRCODPIKNYEAC

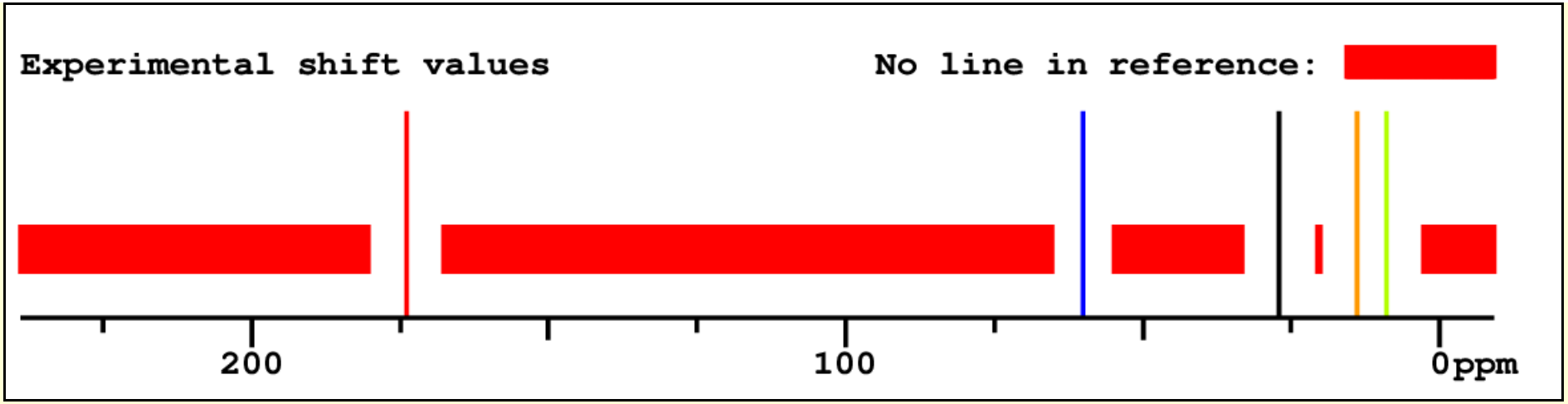
Availability

Predicted Chemical Shiftvalues	Matching Map



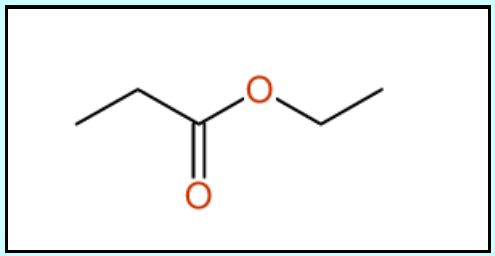
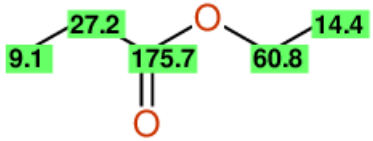
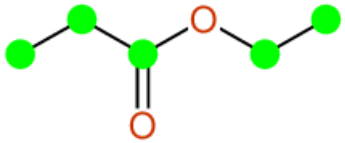


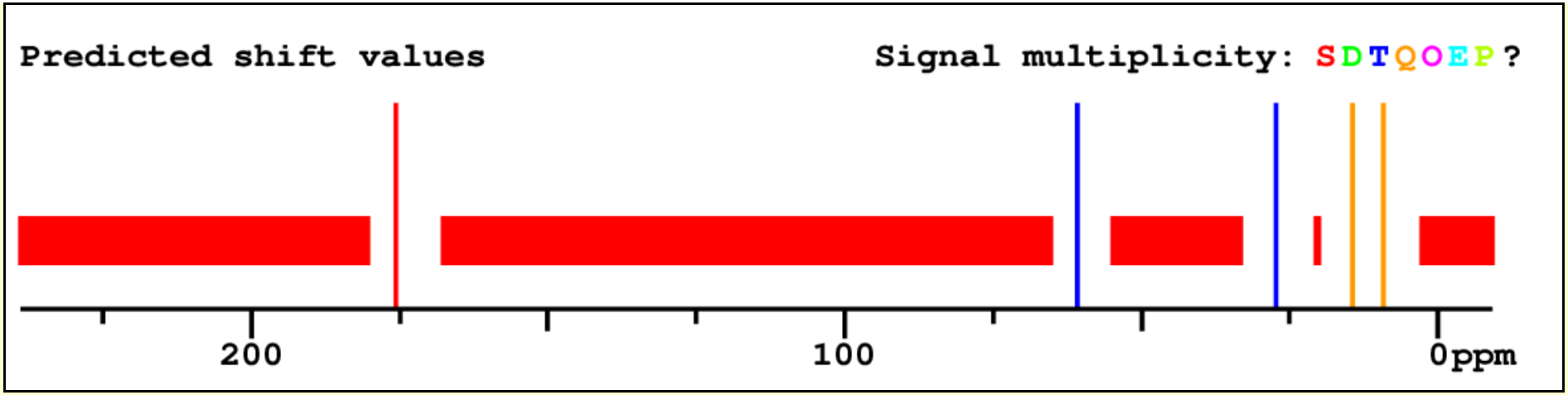


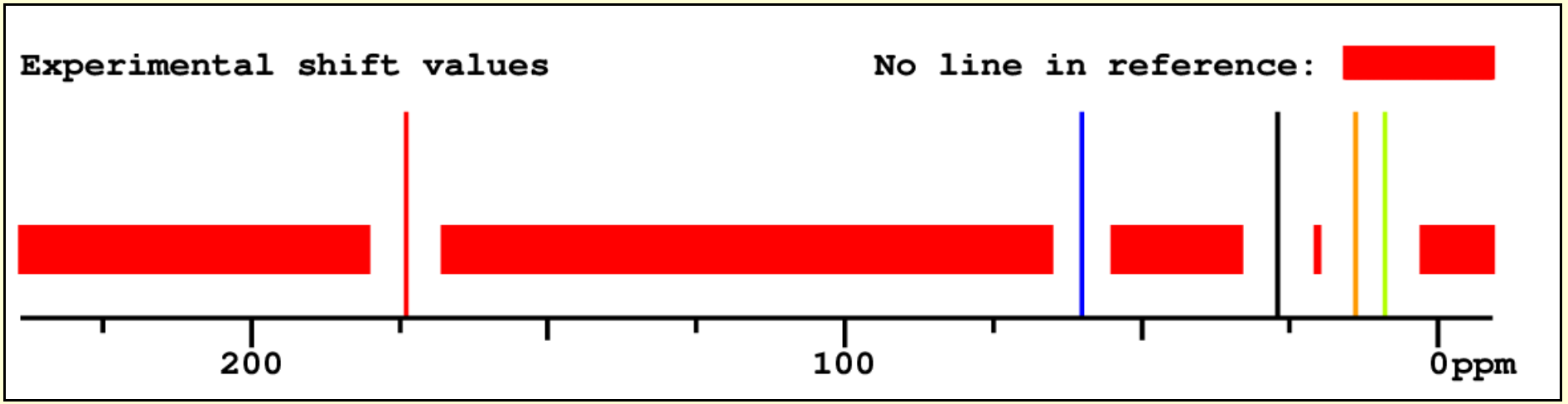


Back to Complete Result

Structure Proposal #2

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_8O_2$ MWT = 100.06 PUBCHEM Search Web for this structure: BYLOWVUCDFUYIQ
Predicted Chemical Shiftvalues	**Matching Map**
	

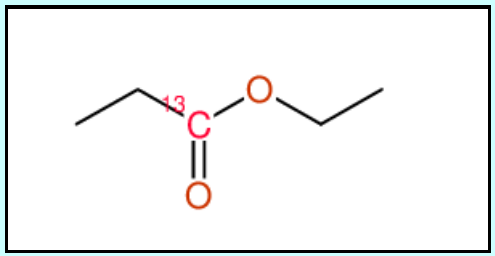




Back to Complete Result

Structure Proposal #3

Structure	Similarity Measure



Deviation = 0.87 ppm

$C_5H_{10}O_2$

MWT = 103.06

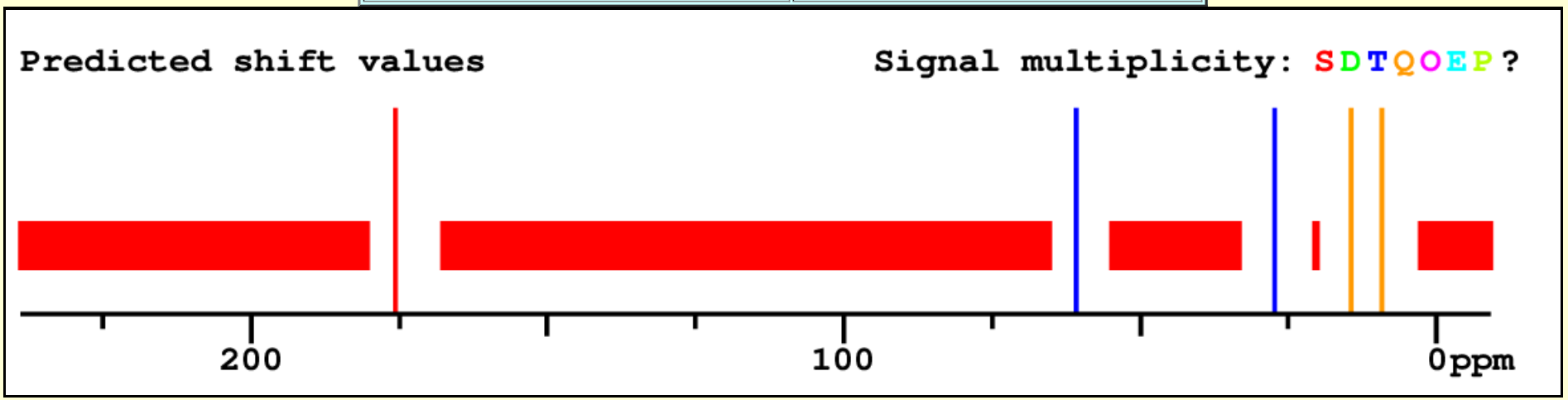
PUBCHEM

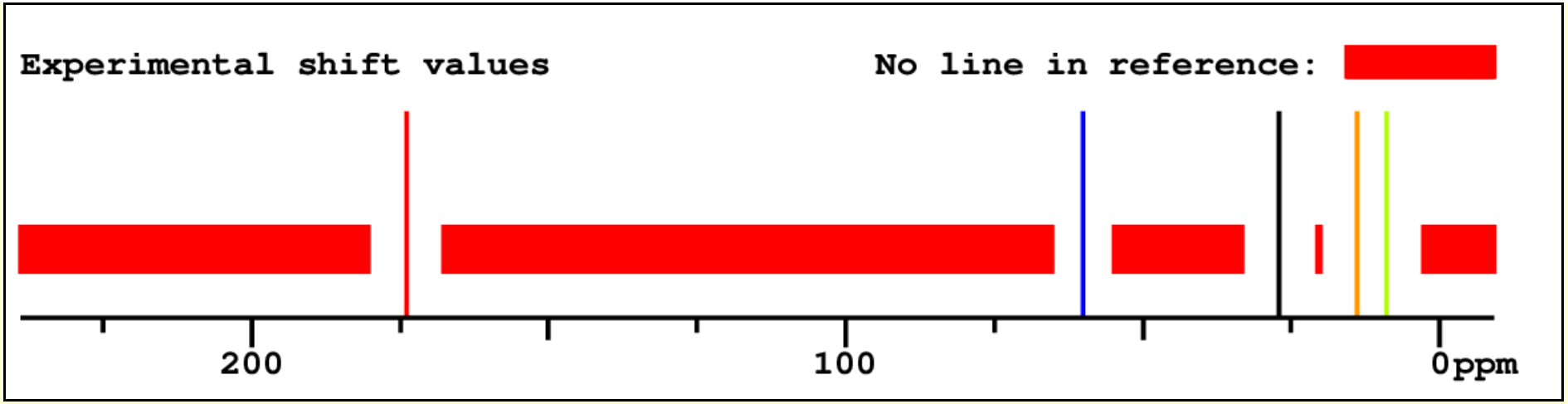
Search Web for this structure:

FKRCODPIKNYEAC

Availability

Predicted Chemical Shiftvalues	Matching Map
	





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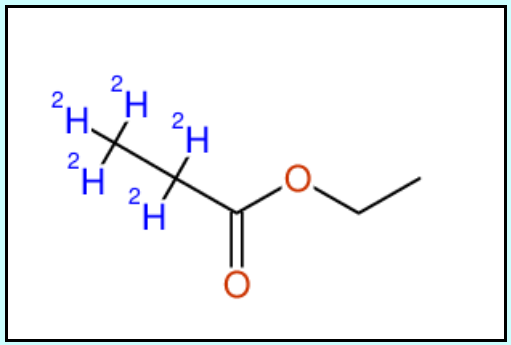
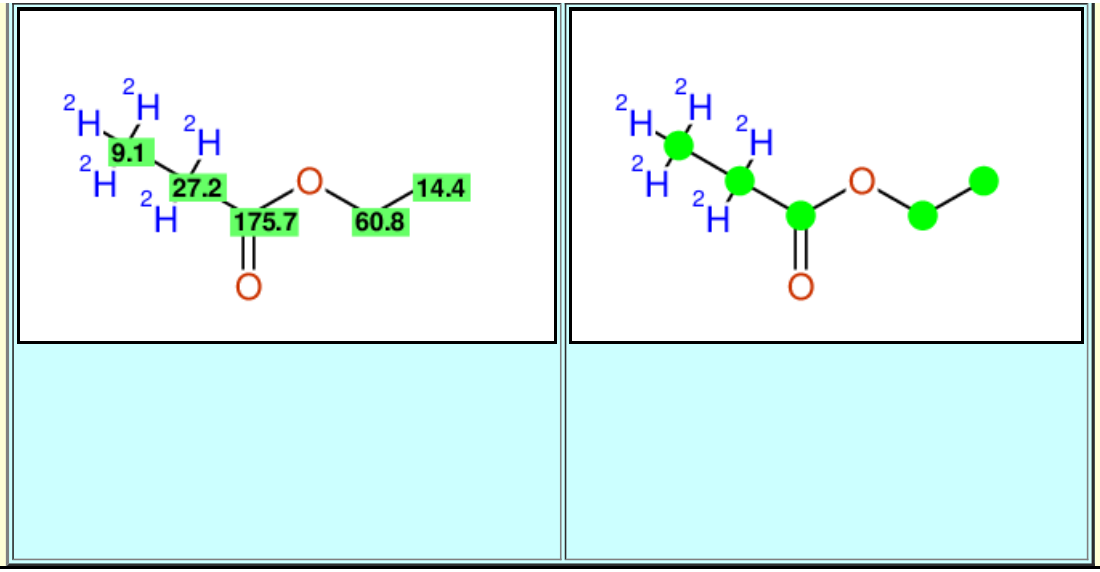
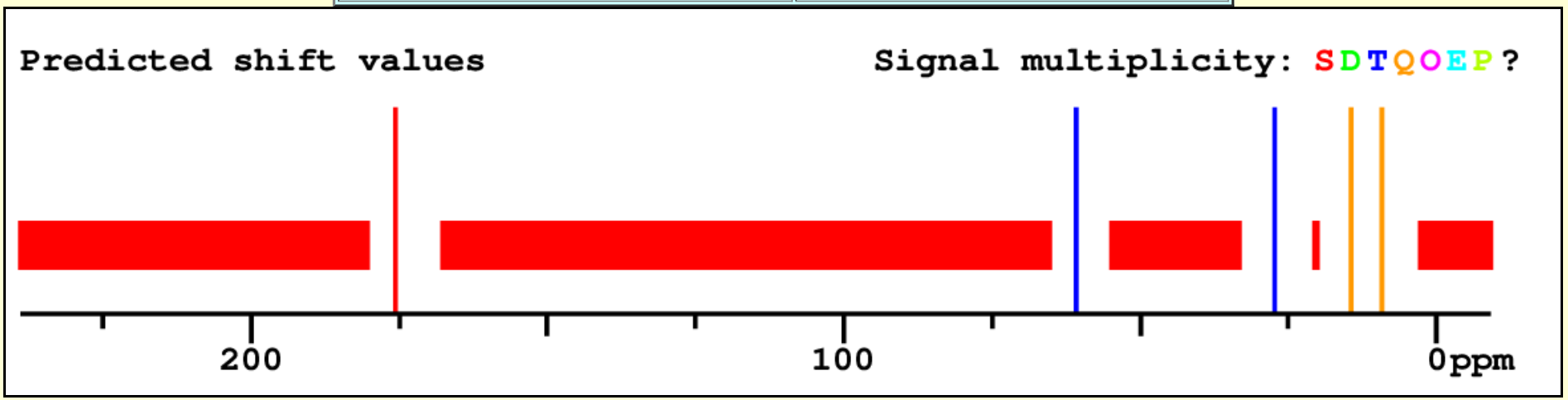
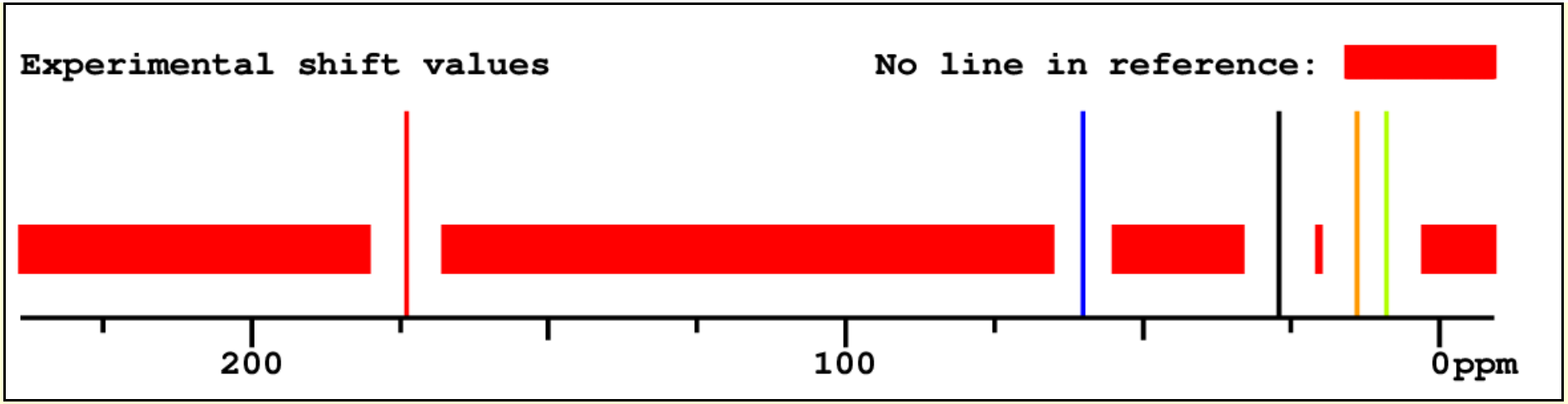
Structure Proposal #4

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_{10}O_2$ MWT = 107.06 PUBCHEM Search Web for this structure: FKRCODPIKNYEAC Availability
Predicted Chemical Shiftvalues	**Matching Map**


9.1
27.2
175.7
60.8
14.4
O
O


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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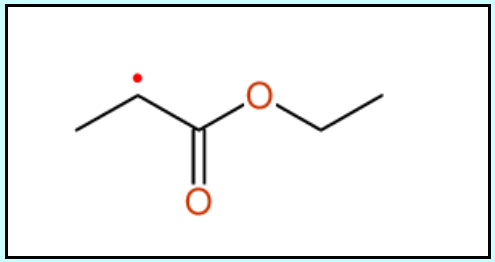
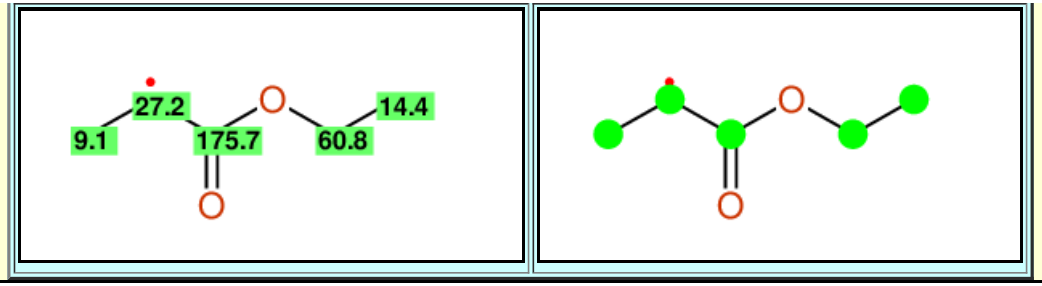
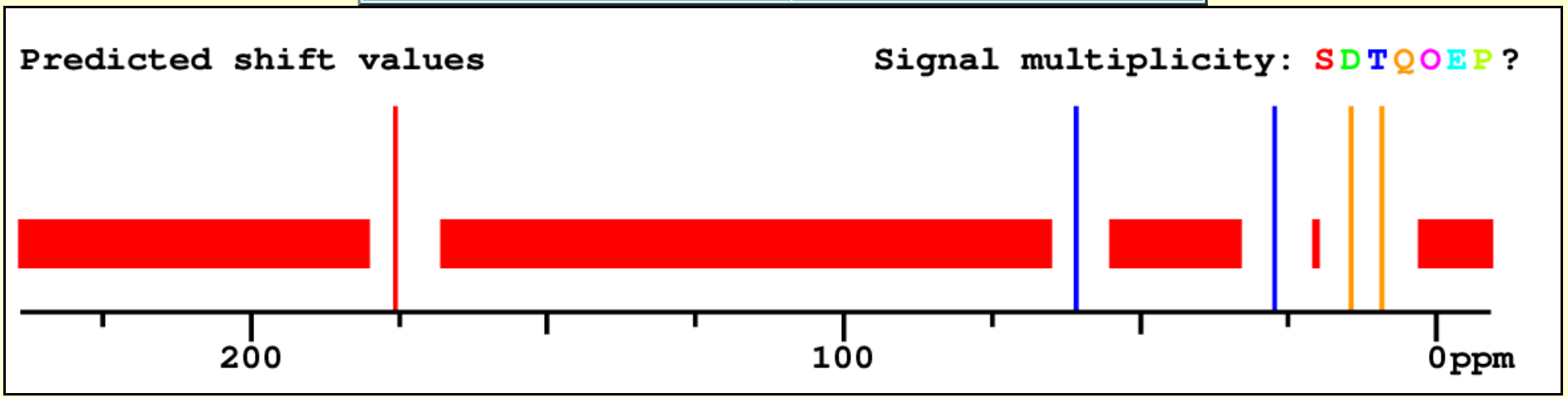
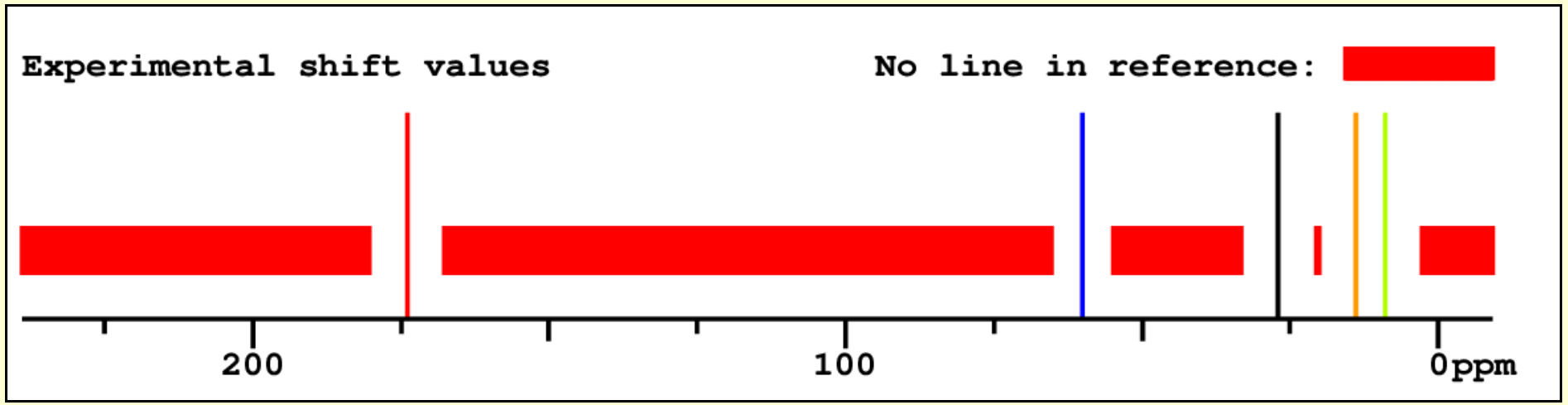
Structure Proposal #5

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_9O_2$ MWT = 101.06 PUBCHEM Search Web for this structure: UPRLWNPAOPKPCE
Predicted Chemical Shiftvalues	Matching Map







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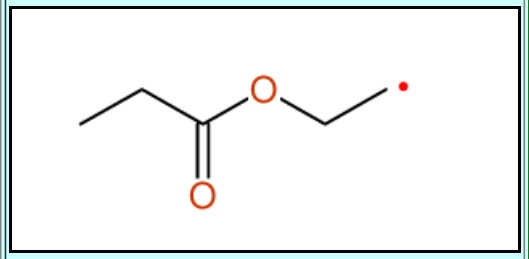
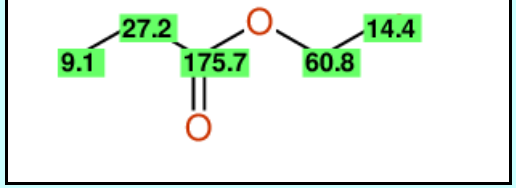
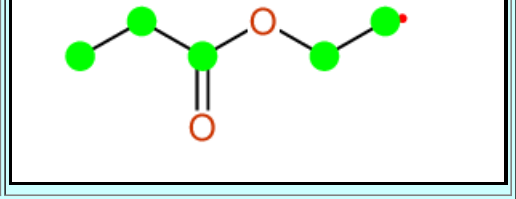
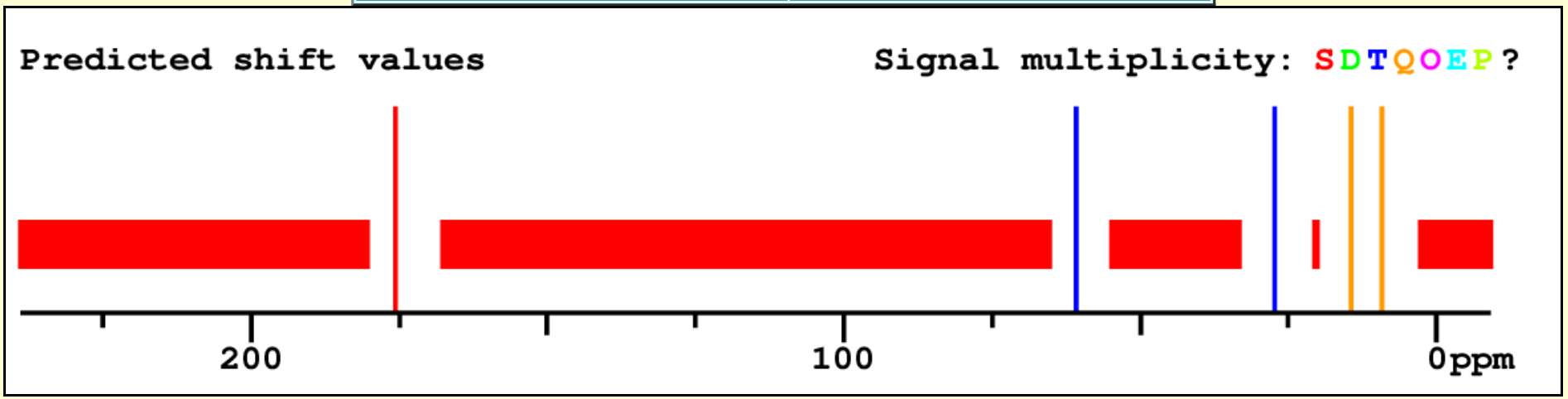
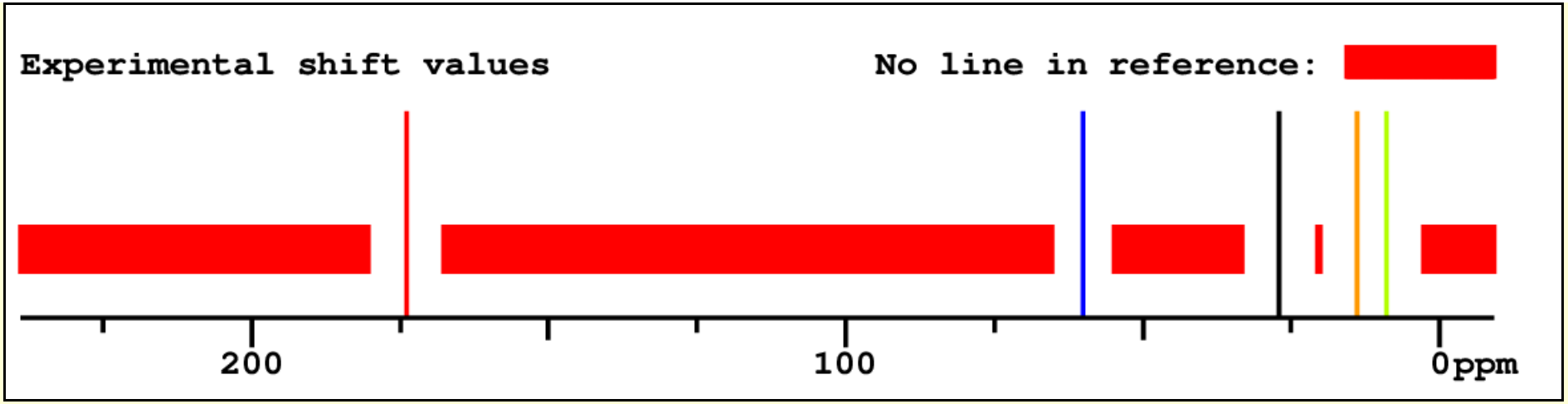
Structure Proposal #6

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_9O_2$ MWT = 101.06 PUBCHEM Search Web for this structure: IRGLFRDZYNBBCO
Predicted Chemical Shiftvalues	**Matching Map**
	





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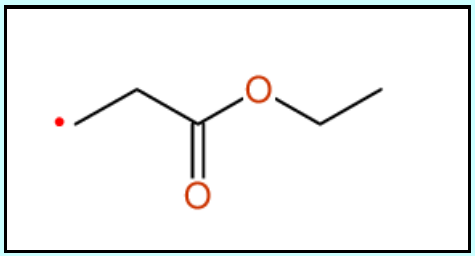
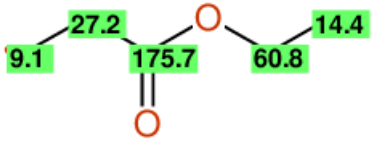
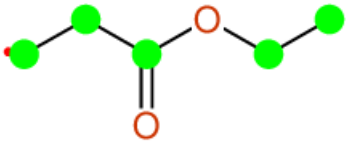
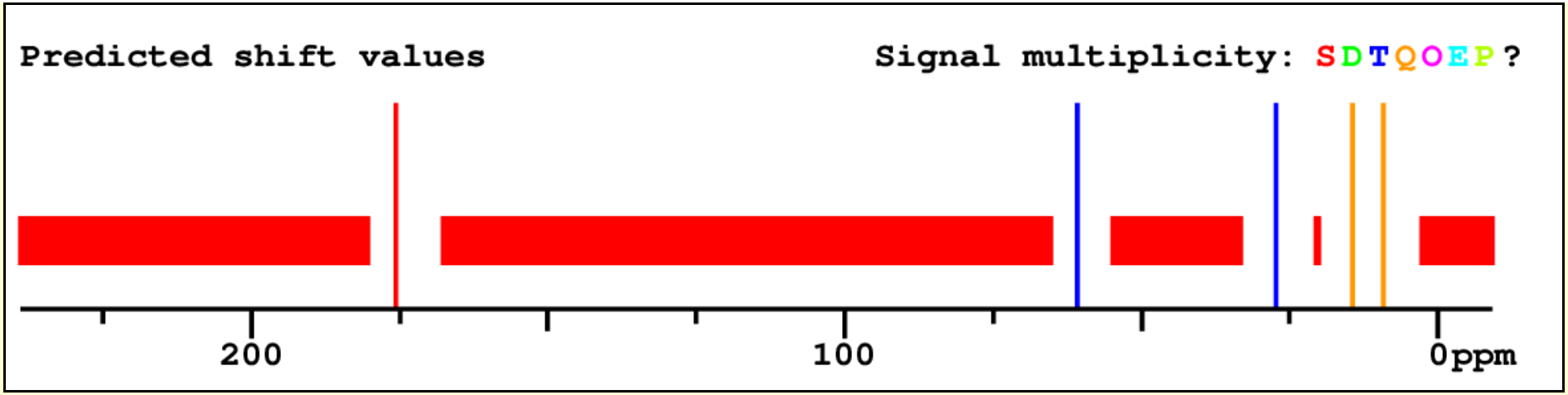
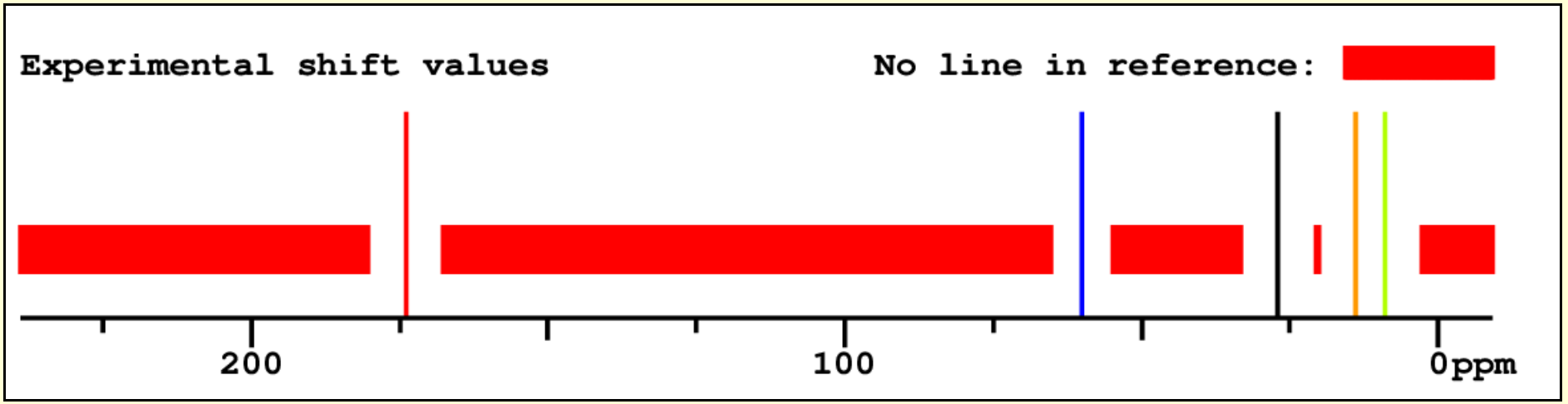
Structure Proposal #7

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_9O_2$ MWT = 101.06 PUBCHEM Search Web for this structure: SQKCNILPACLIRC
Predicted Chemical Shiftvalues	**Matching Map**
	





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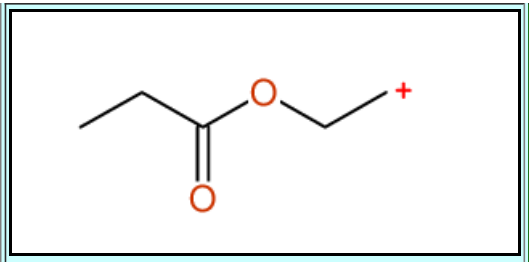
Structure Proposal #8

Structure	Similarity Measure



Deviation = 0.87 ppm

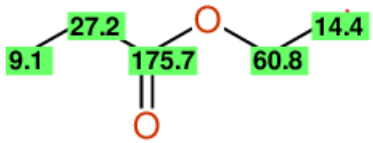
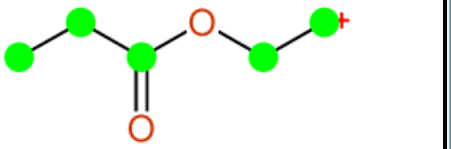
$C_5H_9O_2^+$

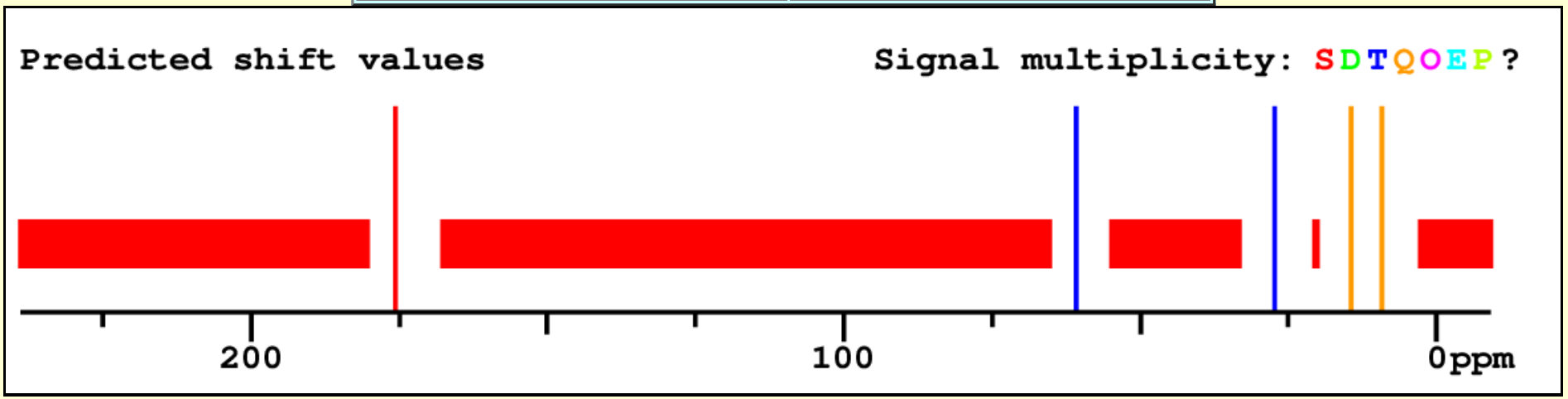
MWT = 101.06

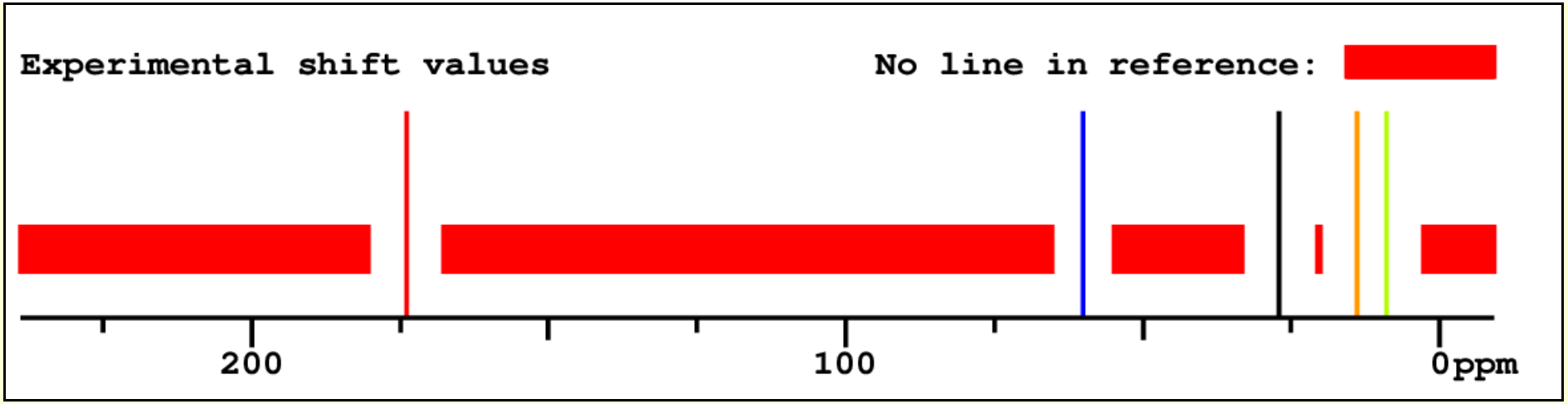
PUBCHEM

Search Web for this structure:

GOKITYWXYBHPKU

Predicted Chemical Shiftvalues	Matching Map
	





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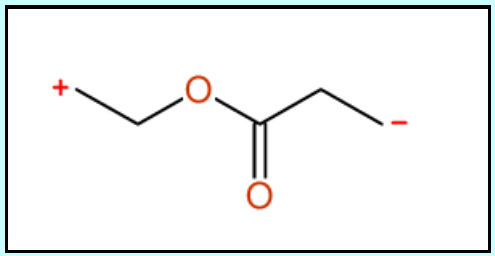
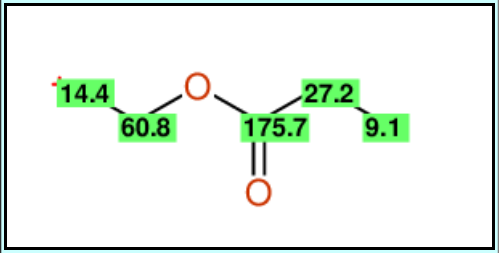
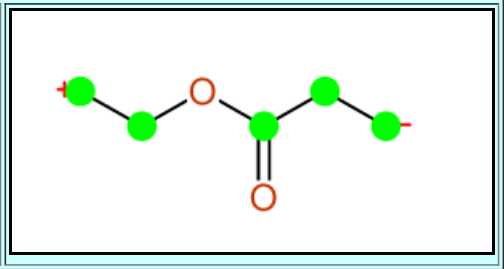
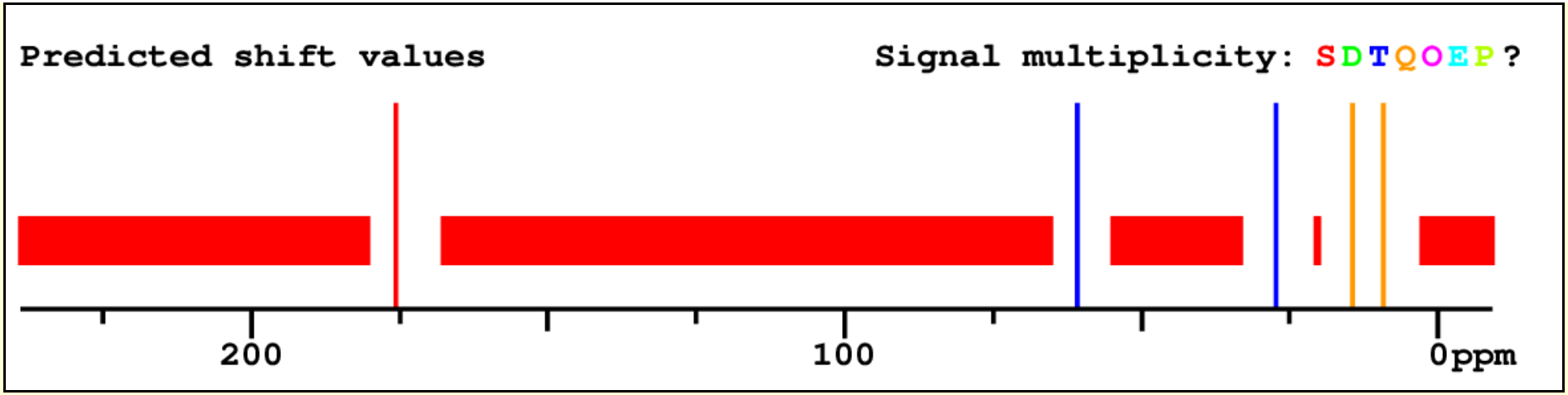
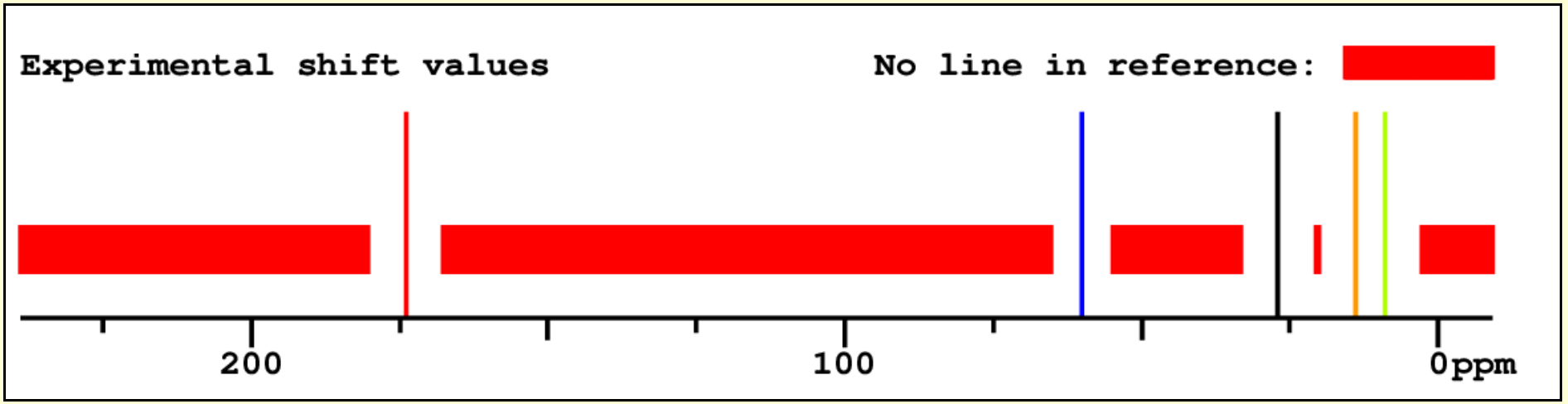
Structure Proposal #9

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_8O_2$ MWT = 100.06 PUBCHEM Search Web for this structure: LVCAAHDUTLIBML
Predicted Chemical Shiftvalues	**Matching Map**
	





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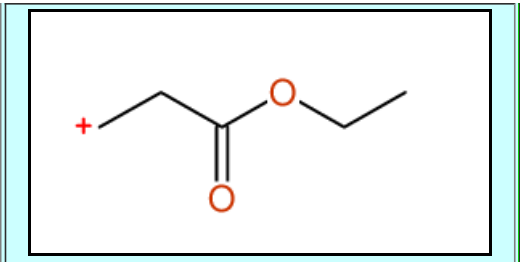
Structure Proposal #10

Structure	Similarity Measure



Deviation = 0.87 ppm

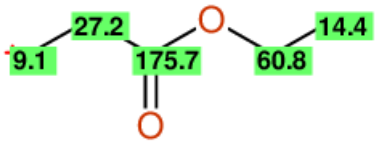
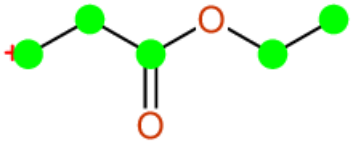
$C_5H_9O_2^+$

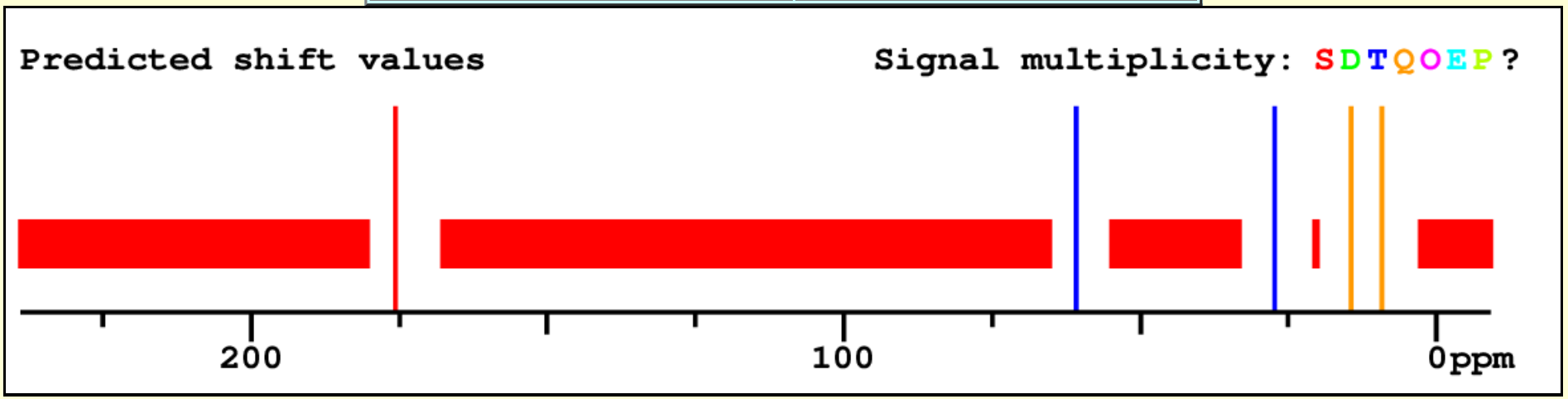
MWT = 101.06

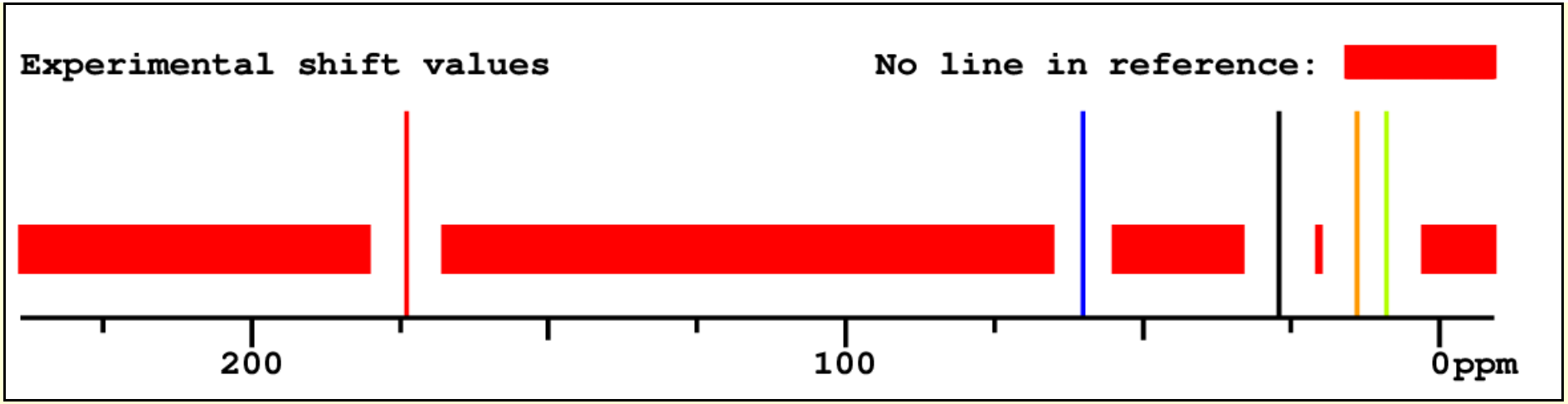
PUBCHEM

Search Web for this structure:

MUQMZQYQIIZBIT

Predicted Chemical Shiftvalues	Matching Map
	





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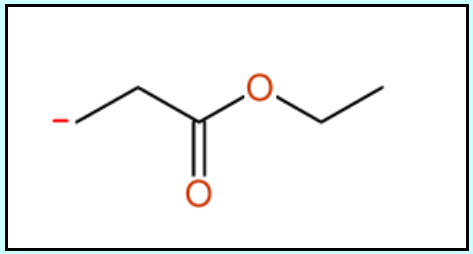
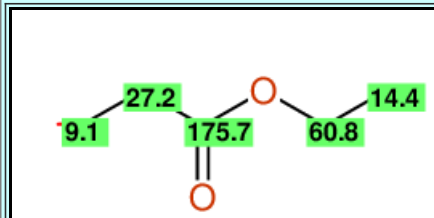
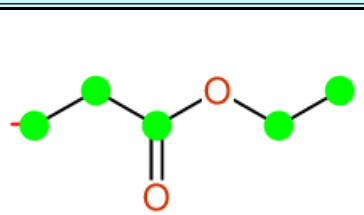
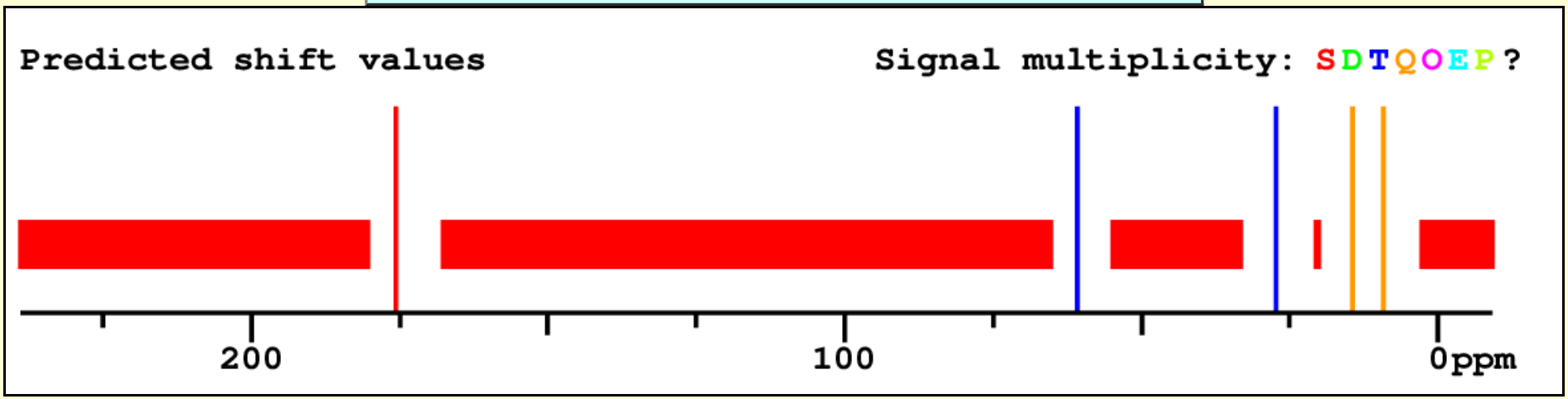
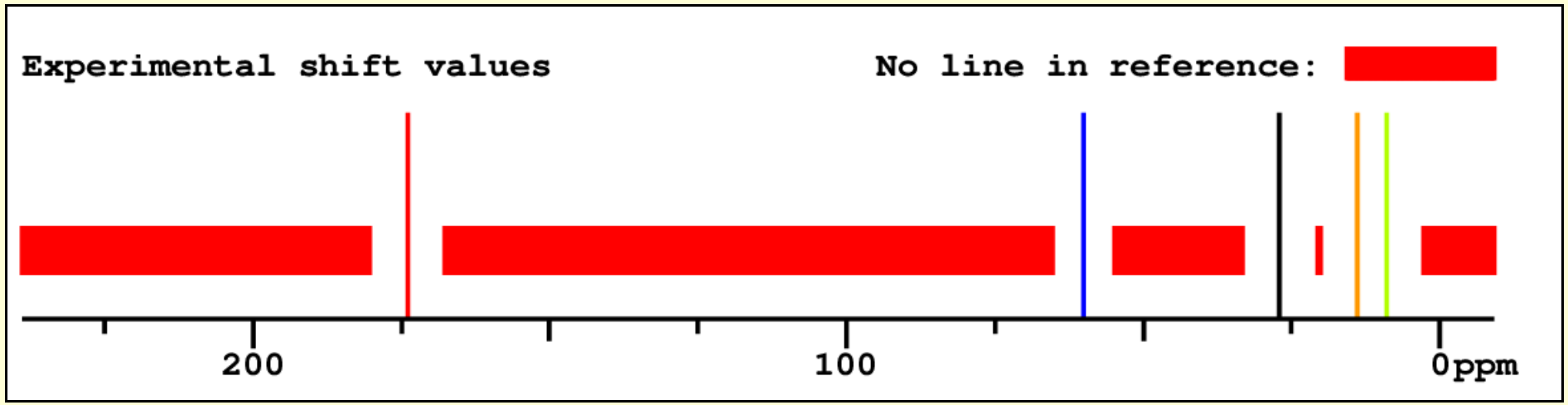
Structure Proposal #11

Structure	Similarity Measure
	Deviation = 0.87 ppm $C_5H_9O_2^-$ MWT = 101.06 PUBCHEM Search Web for this structure: NWIUUTFORIXPJC
Predicted Chemical Shiftvalues	**Matching Map**
	





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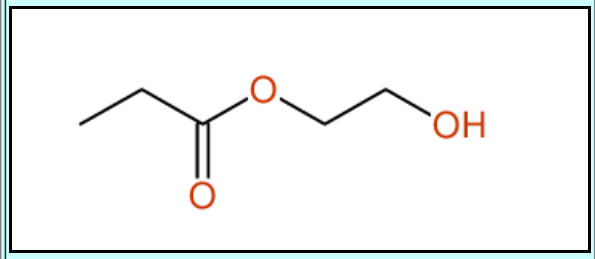
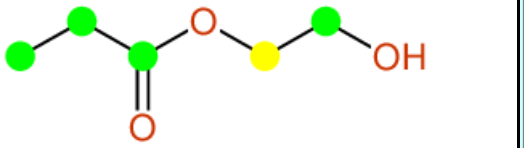
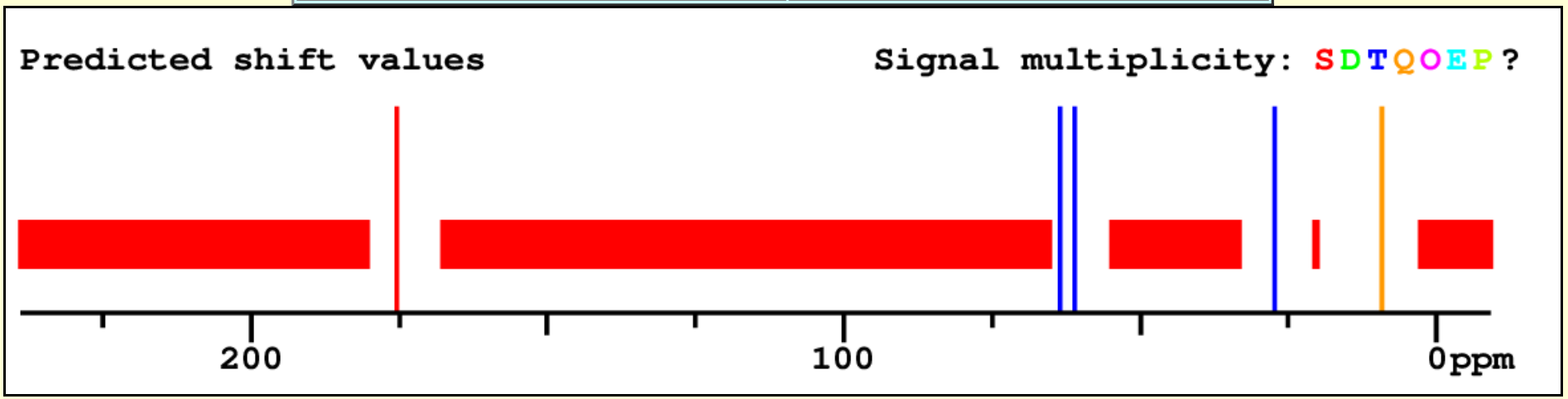
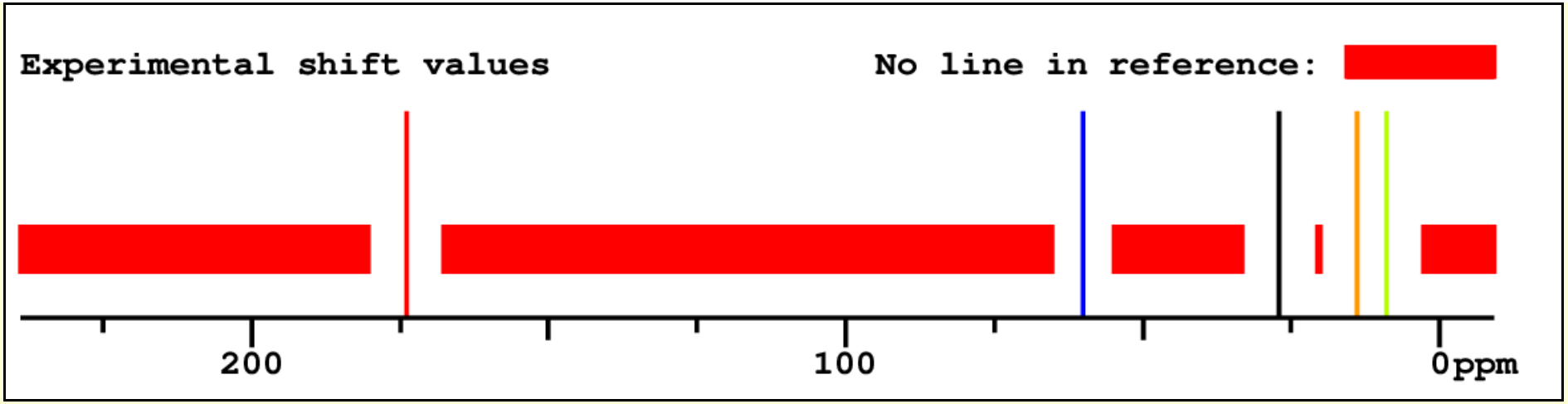
Structure Proposal #12

Structure	Similarity Measure
	Deviation = 2.02 ppm $C_5H_{10}O_3$ MWT = 118.06 PUBCHEM Search Web for this structure: SFAMKDPMPDEXGH
Predicted Chemical Shiftvalues	**Matching Map**
	





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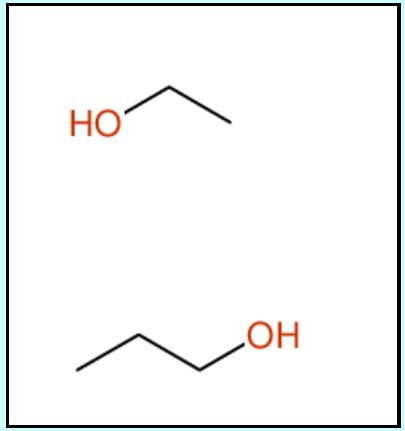
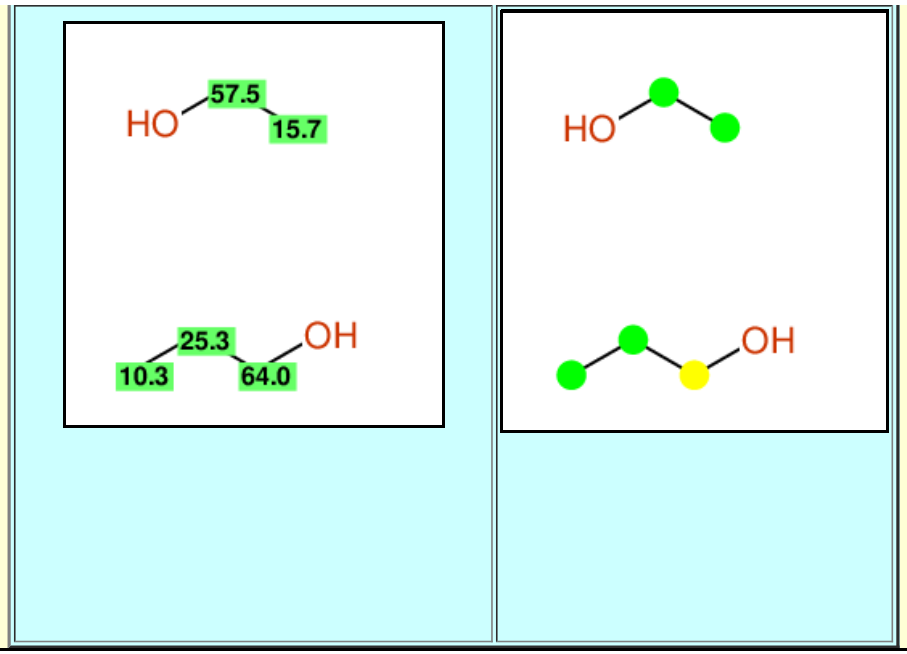
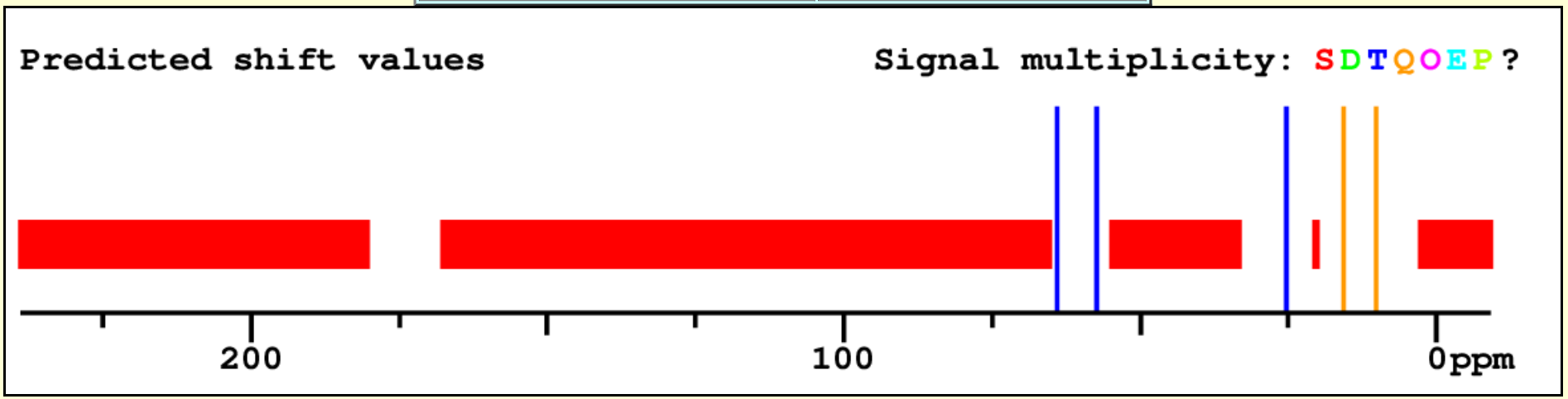
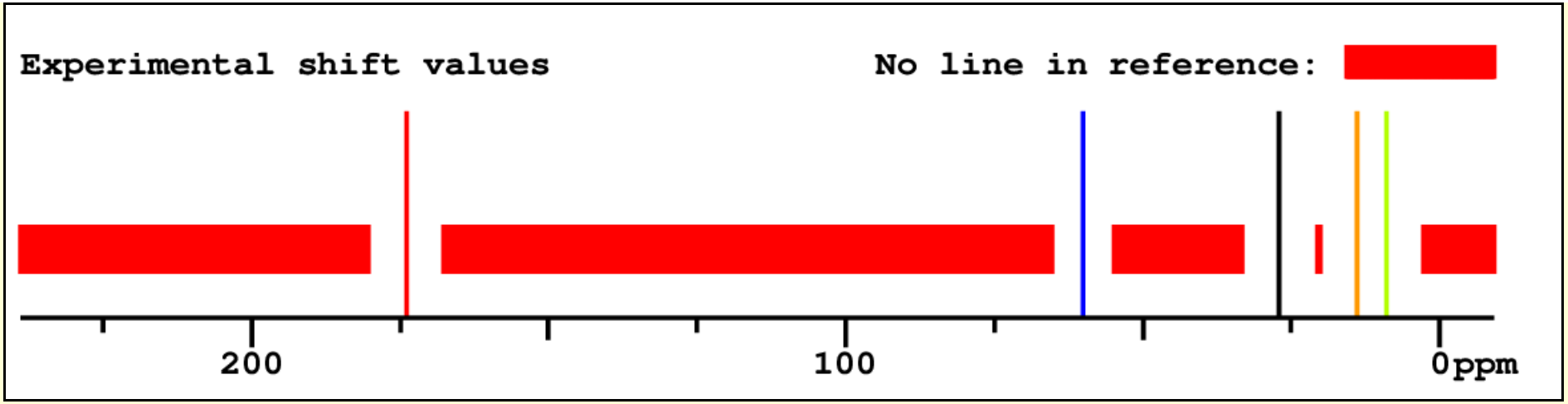
Structure Proposal #13

Structure	Similarity Measure
	Deviation = 2.62 ppm $C_5H_{14}O_2$ MWT = 106.06 PUBCHEM Search Web for this structure: OMRDZQXXMYCHBU
Predicted Chemical Shiftvalues	Matching Map


HO
57.5
15.7
25.3
OH
10.3
64.0
HO
OH


Predicted shift values
Signal multiplicity: SDTQQOEP?
200
100
0ppm



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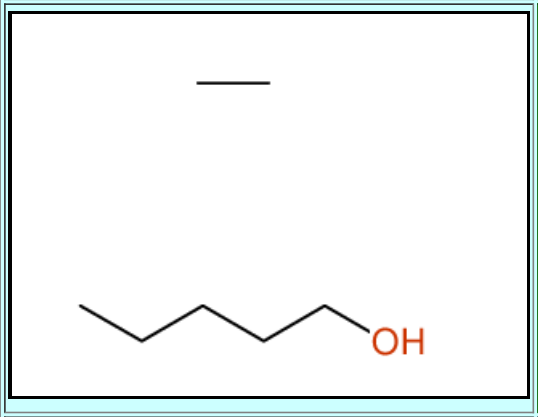
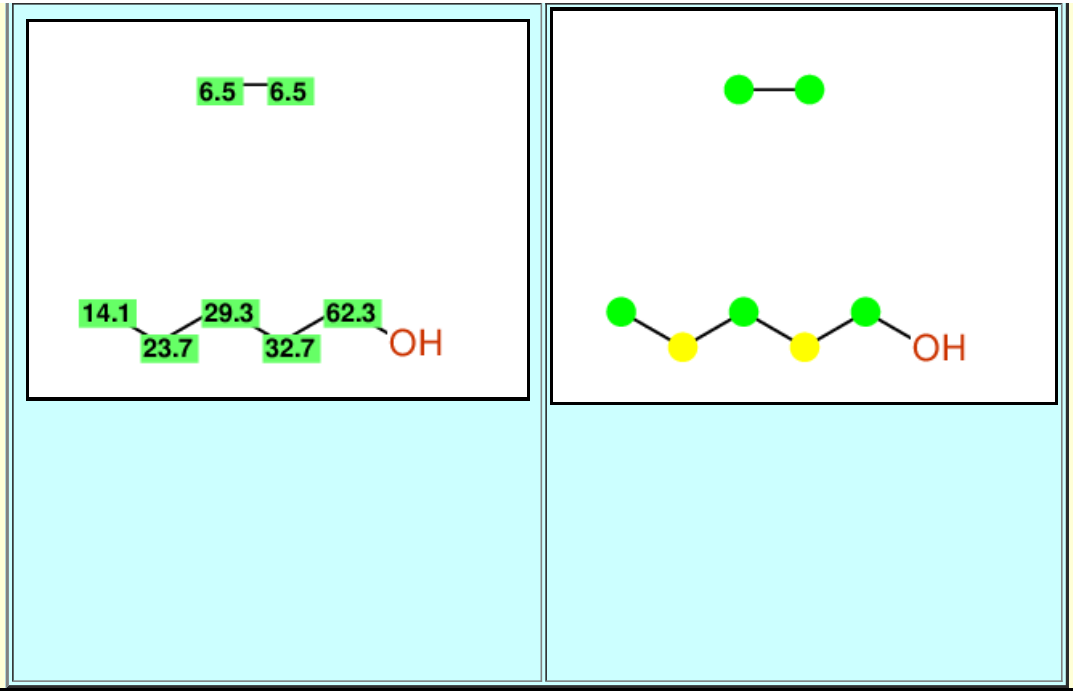
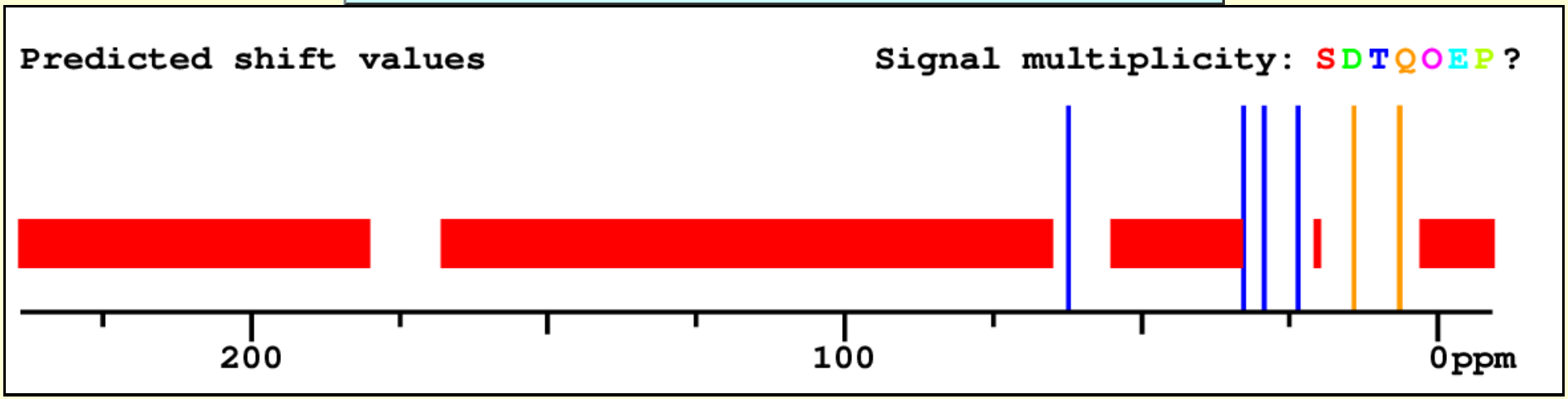
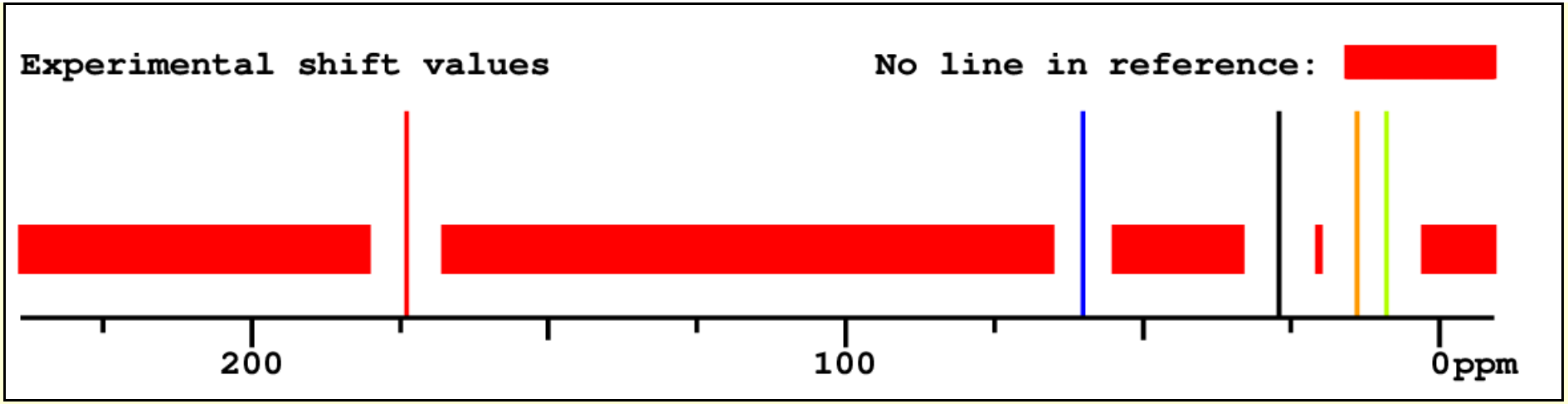
Structure Proposal #14

Structure	Similarity Measure
	Deviation = 2.98 ppm $C_7H_{18}O$ MWT = 118.08 PUBCHEM Search Web for this structure: ZARMDFHSJSIZKQ
Predicted Chemical Shiftvalues	**Matching Map**


6.5
6.5
14.1
23.7
29.3
32.7
62.3
OH
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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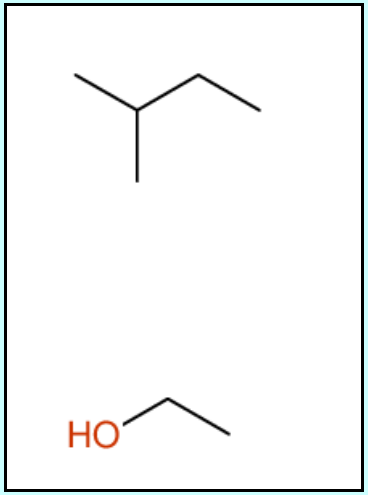
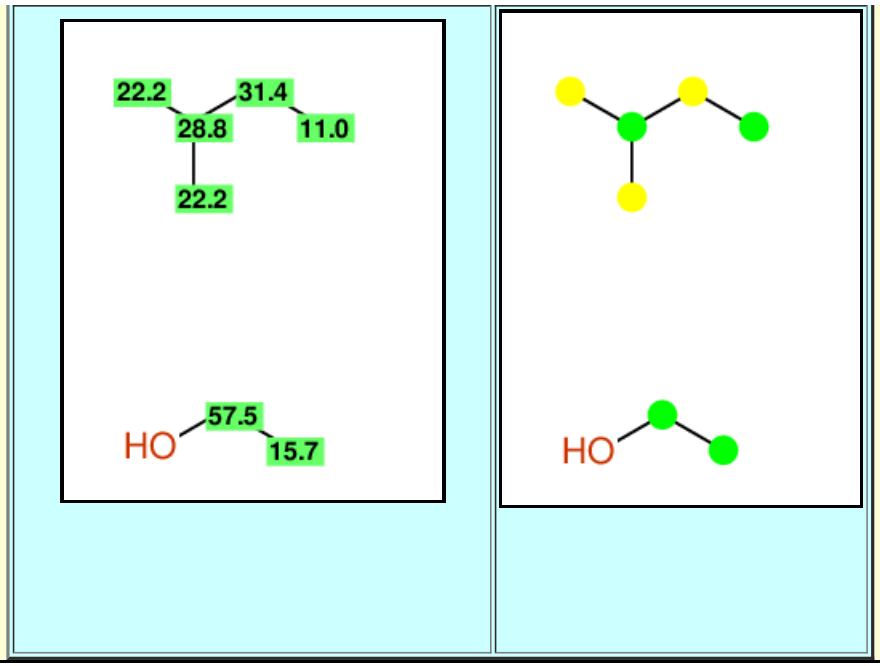
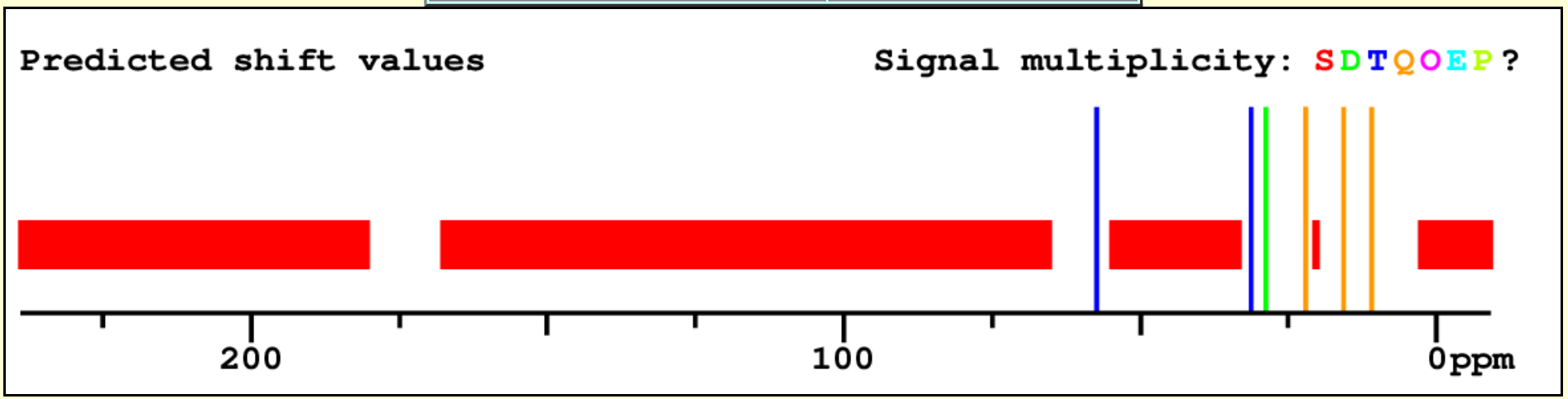
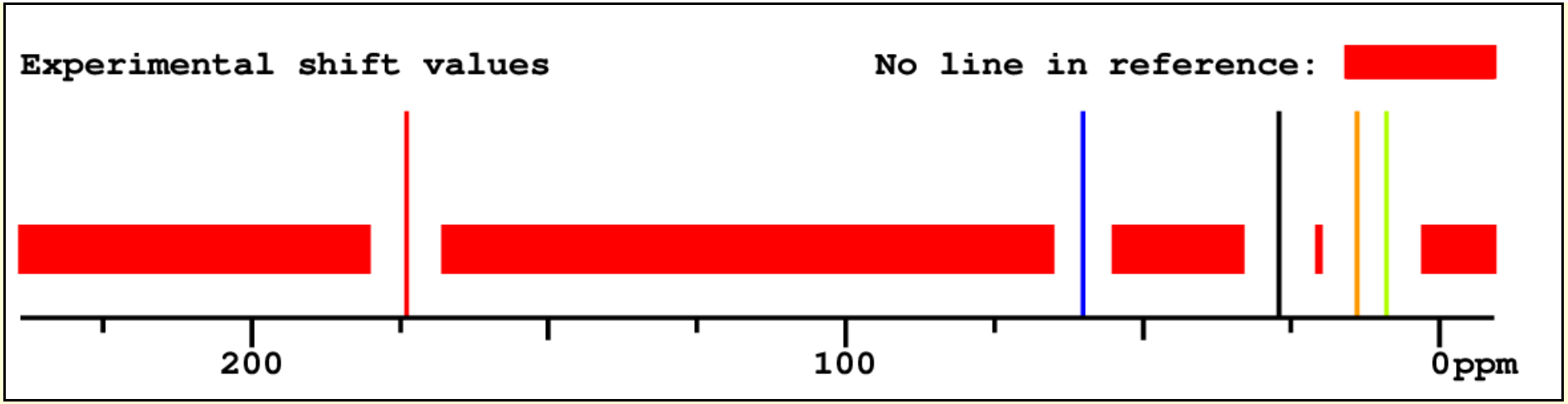
Structure Proposal #15

Structure	Similarity Measure
	Deviation = 3.16 ppm $C_7H_{18}O$ MWT = 118.08 PUBCHEM Search Web for this structure: FOXQTCHXXJKLNK
Predicted Chemical Shiftvalues	**Matching Map**


22.2
31.4
28.8
11.0
22.2
57.5
HO
15.7
HO


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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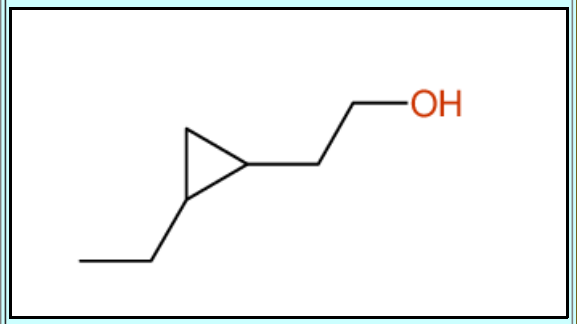
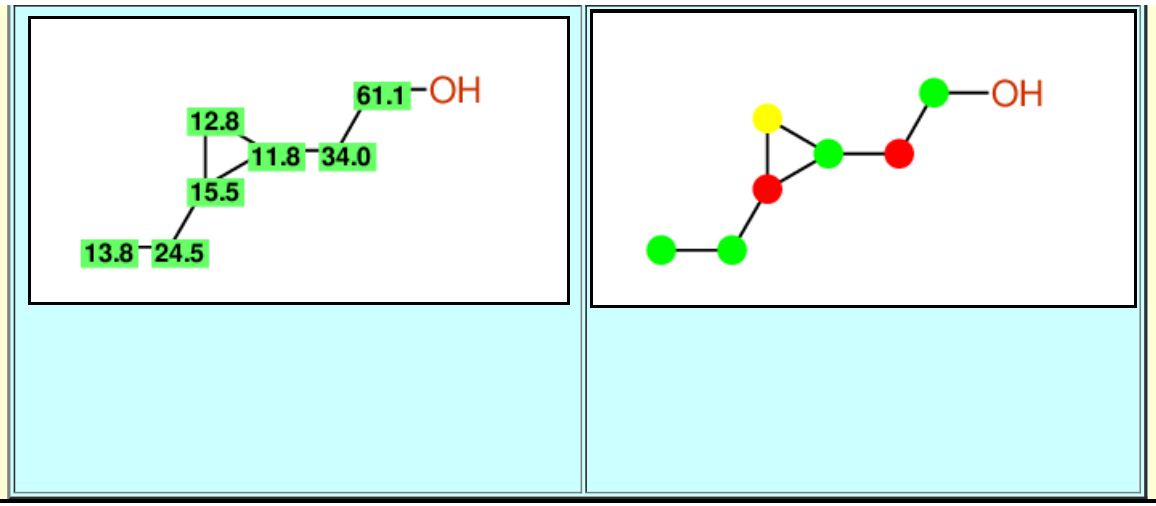
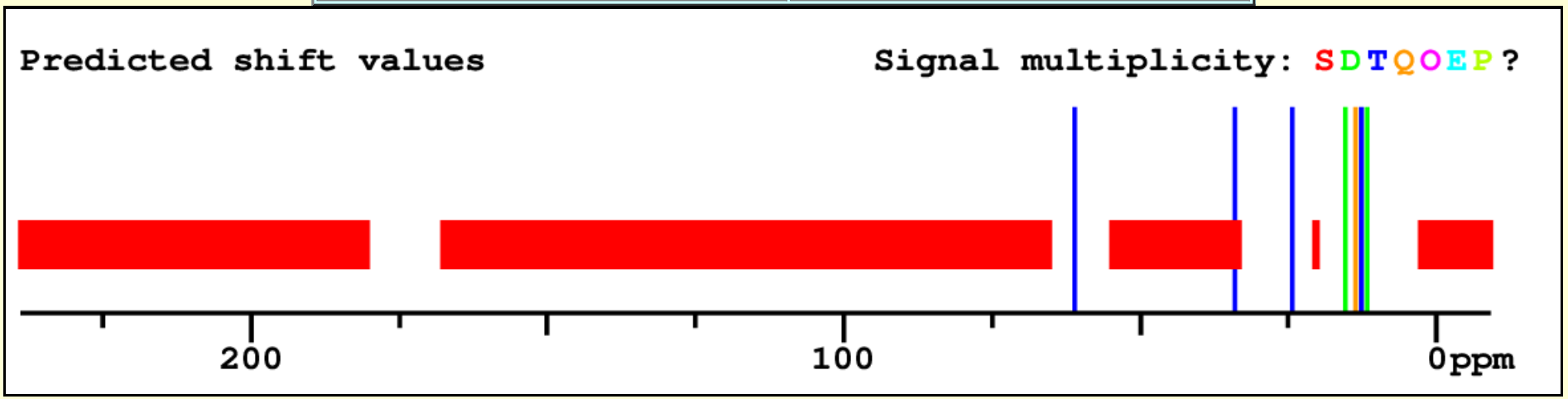
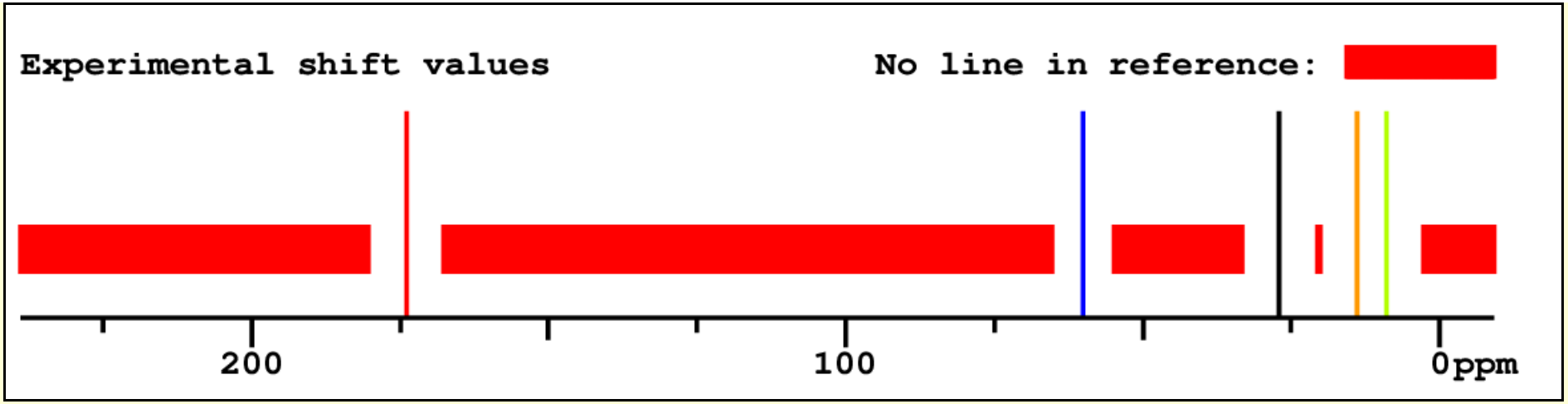
Structure Proposal #16

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


61.1
OH
12.8
11.8
34.0
15.5
13.8
24.5
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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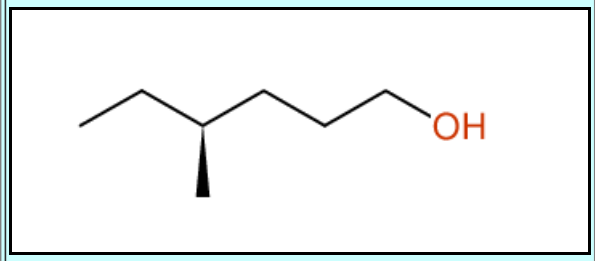
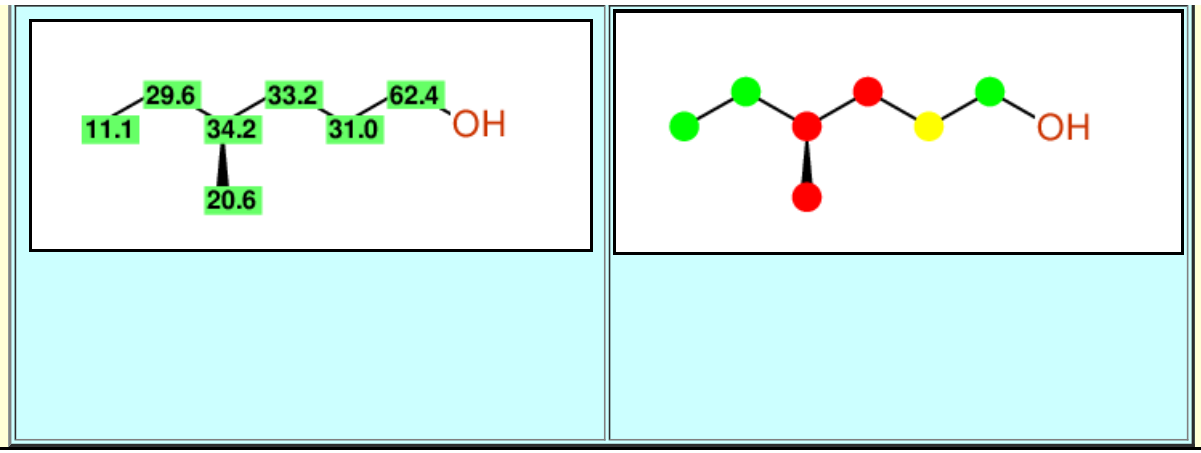
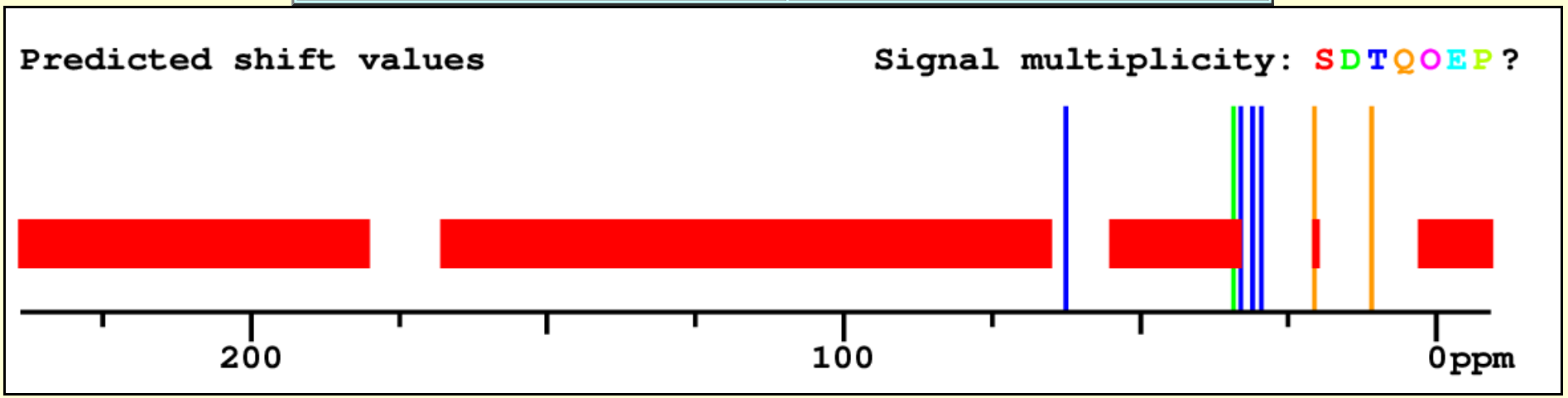
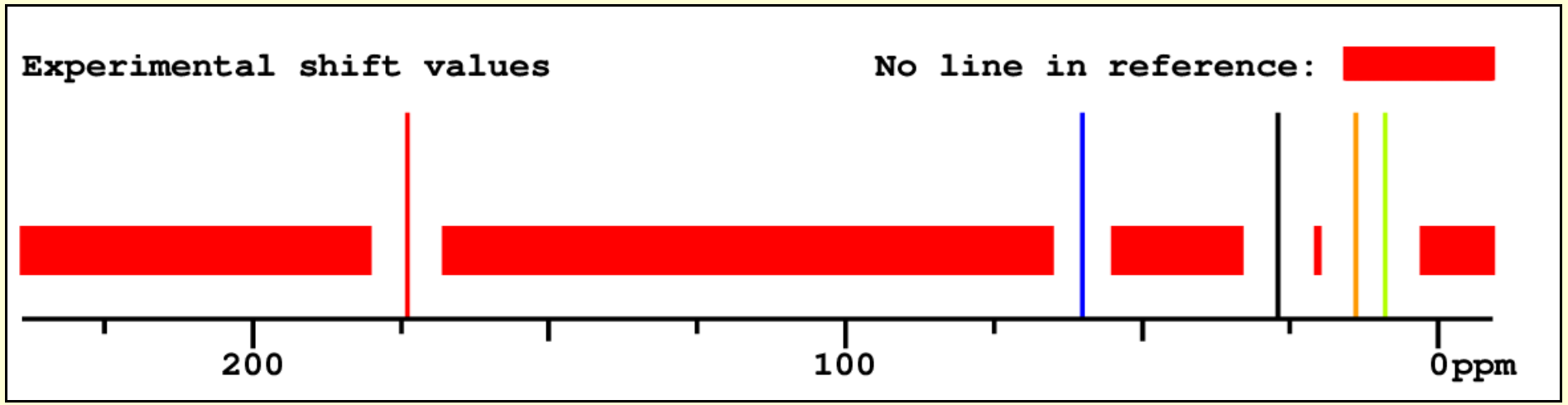
Structure Proposal #17

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


29.6
33.2
62.4
11.1
34.2
31.0
OH
20.6
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm


Experimental shift values
No line in reference:
200
100
0ppm

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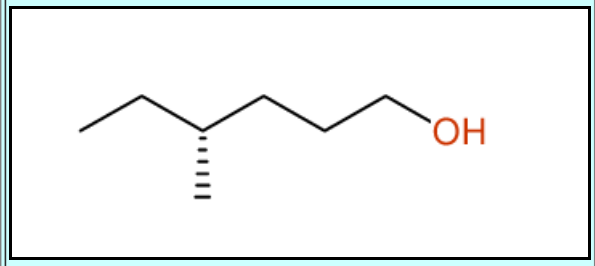
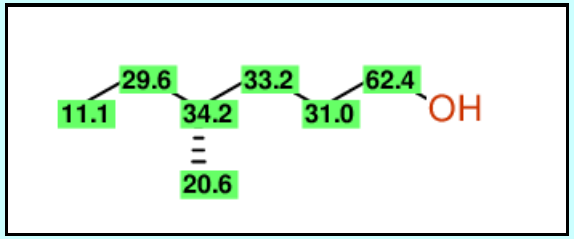
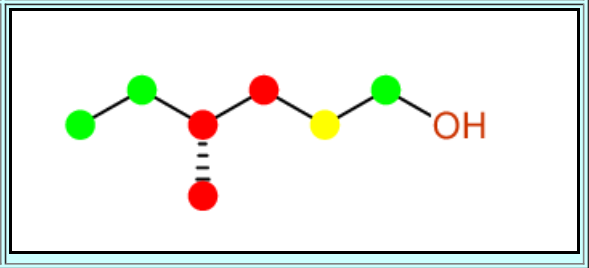
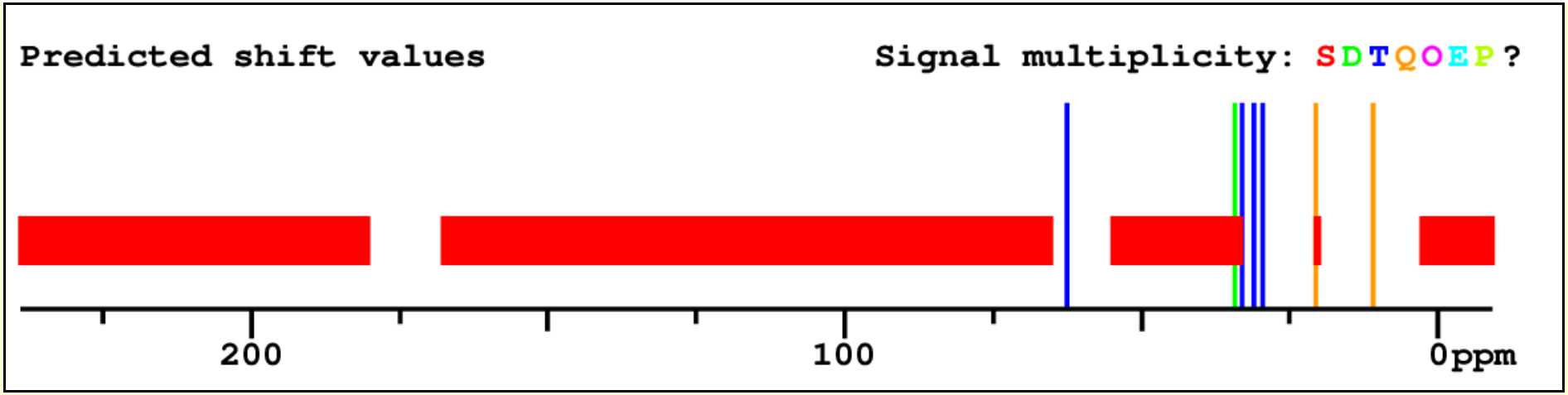
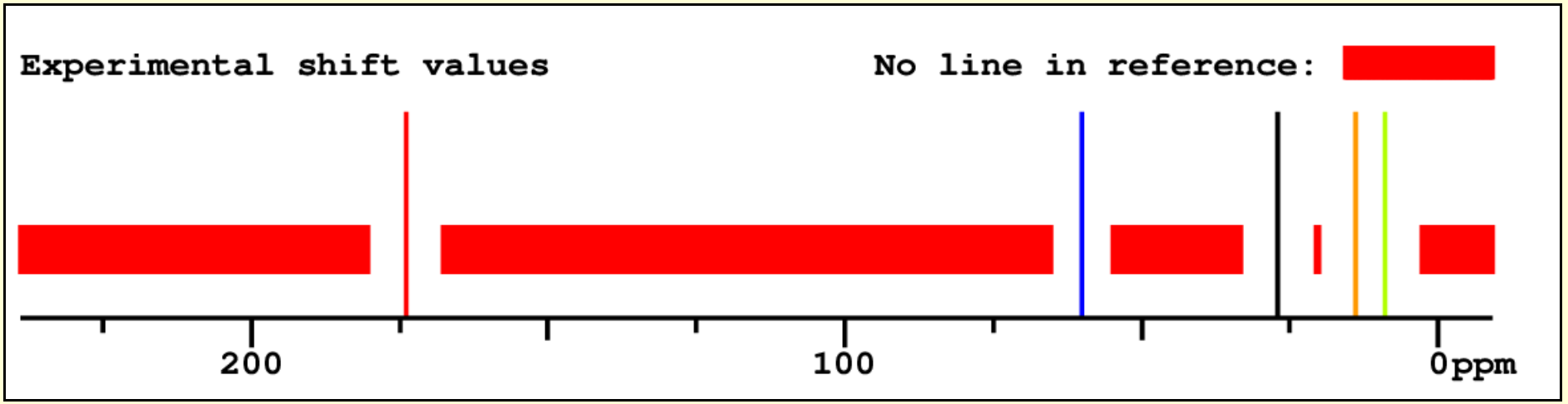
Structure Proposal #18

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





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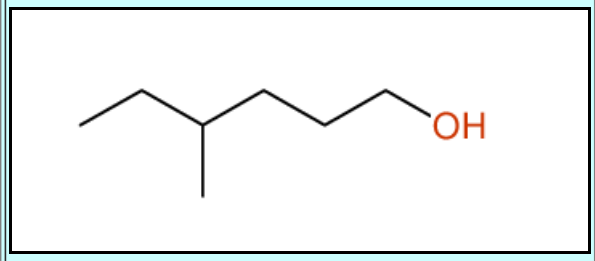
Structure Proposal #19

Structure	Similarity Measure



Deviation = 4.01 ppm
(Different pattern)

$C_7H_{16}O$

MWT = 116.08

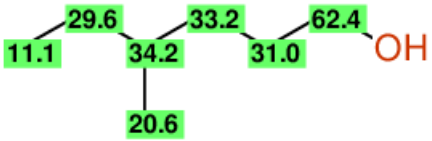
PUBCHEM

Search Web for this structure:

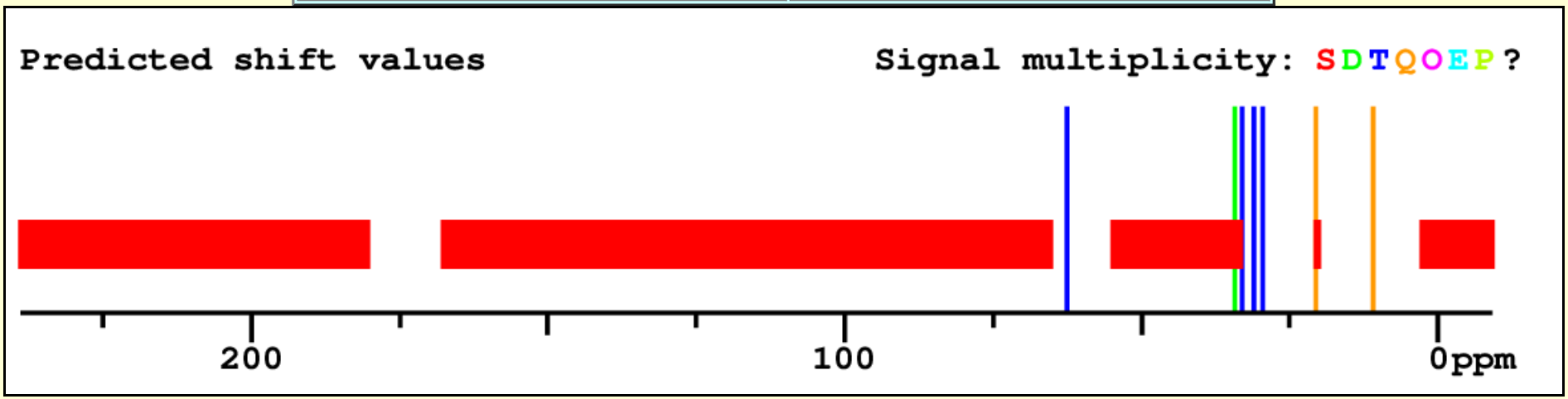
YNPVNLWKVZZBTM

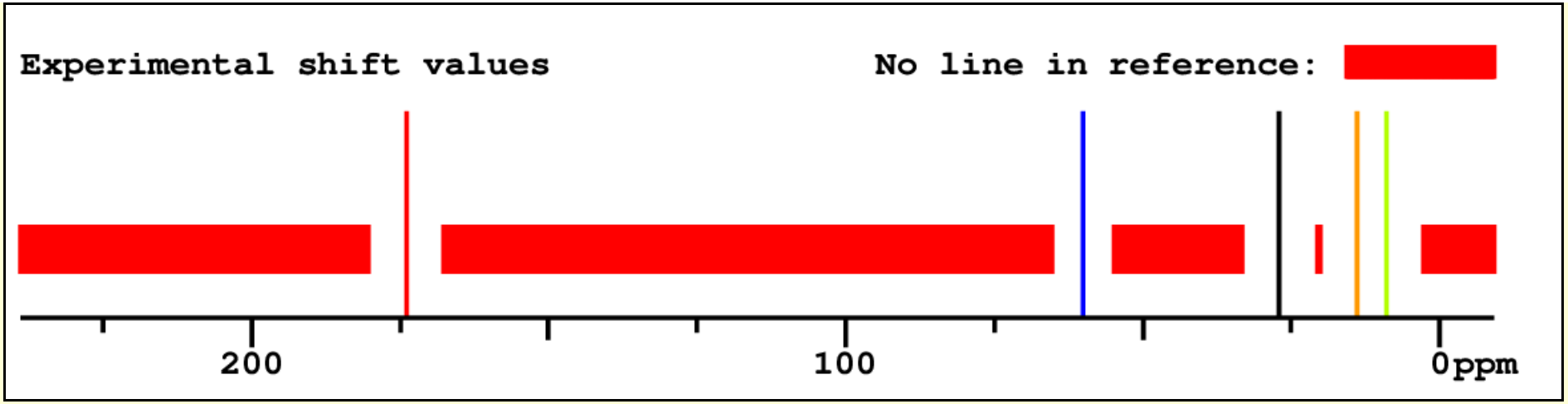
Availability

Predicted Chemical Shiftvalues



Matching Map





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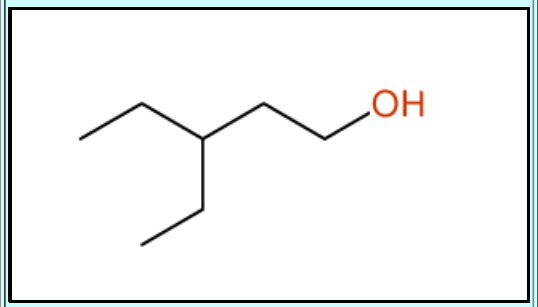
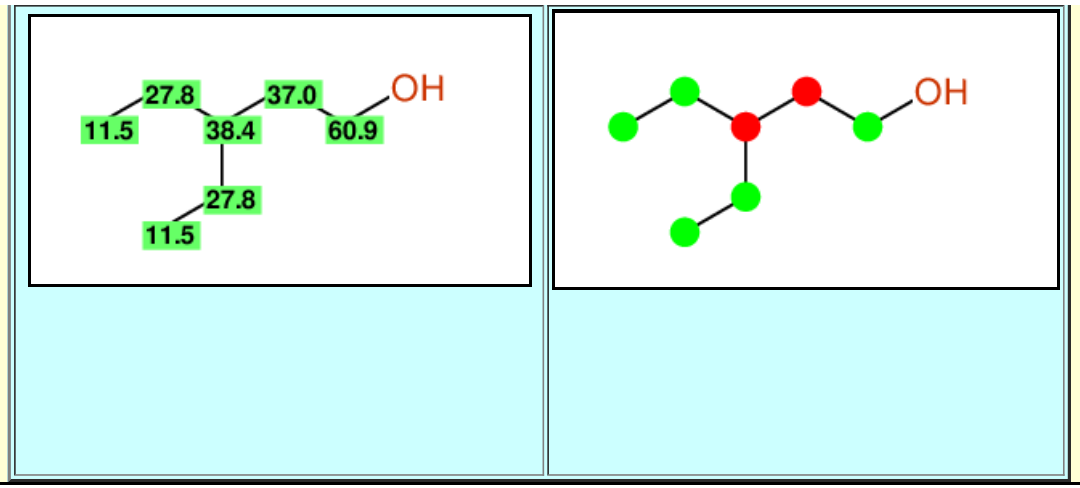
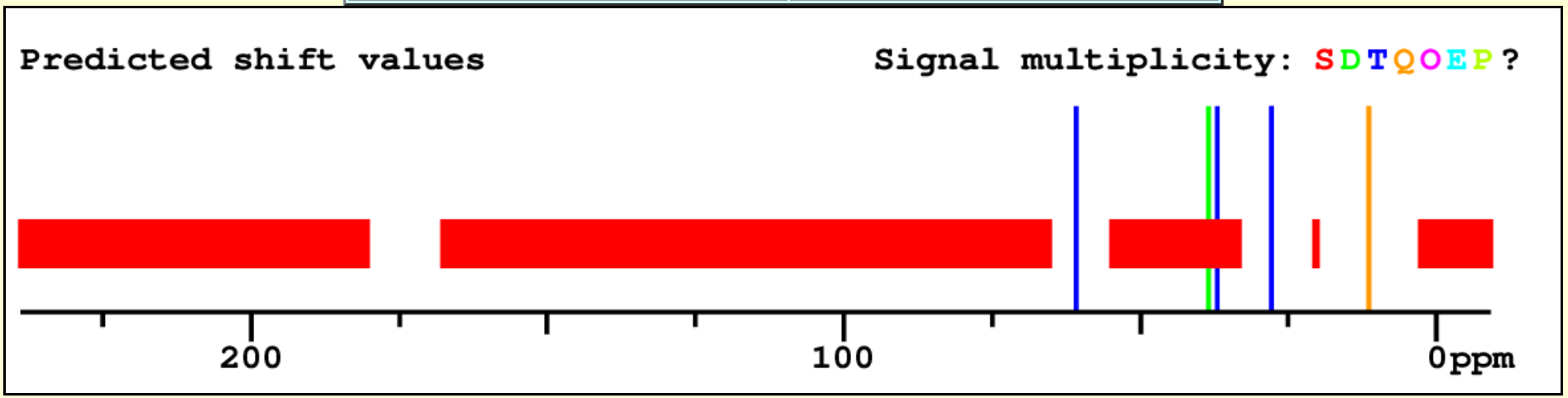
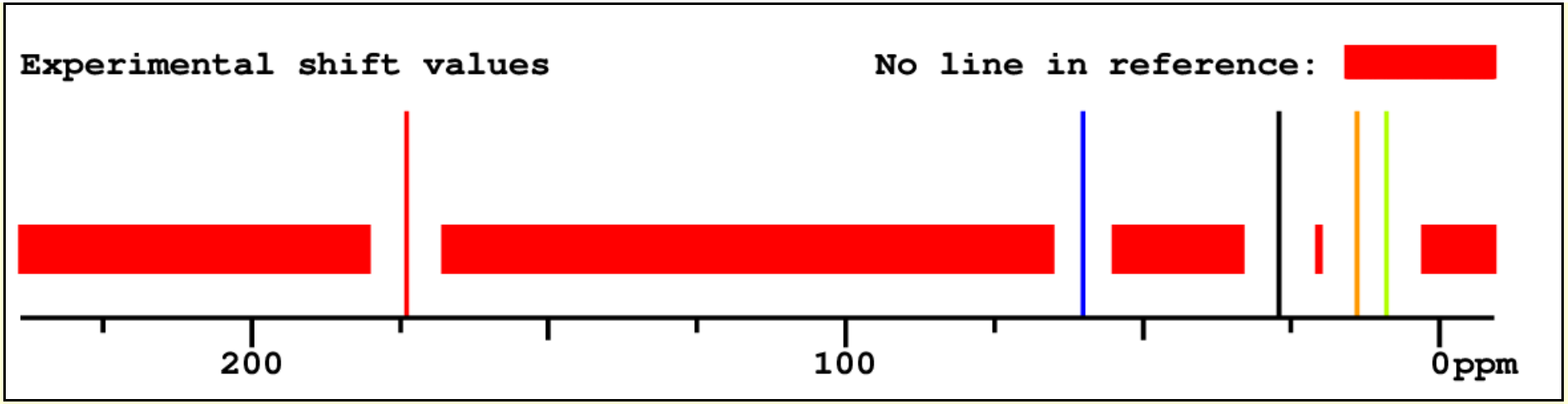
Structure Proposal #20

Structure	Similarity Measure
	**Deviation = 4.36 ppm** (Different pattern) **$C_7H_{16}O$** **MWT = 116.08** **PUBCHEM** **Search Web for this structure:** **DVEFUHVVWJONKR** Availability
Predicted Chemical Shiftvalues	**Matching Map**


27.8
37.0
OH
11.5
38.4
60.9
27.8
11.5
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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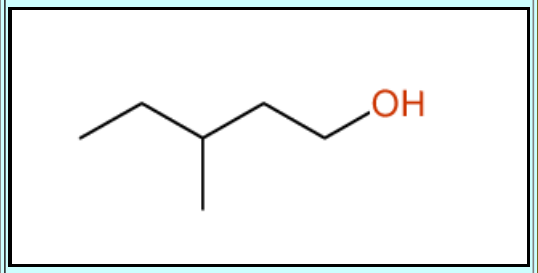
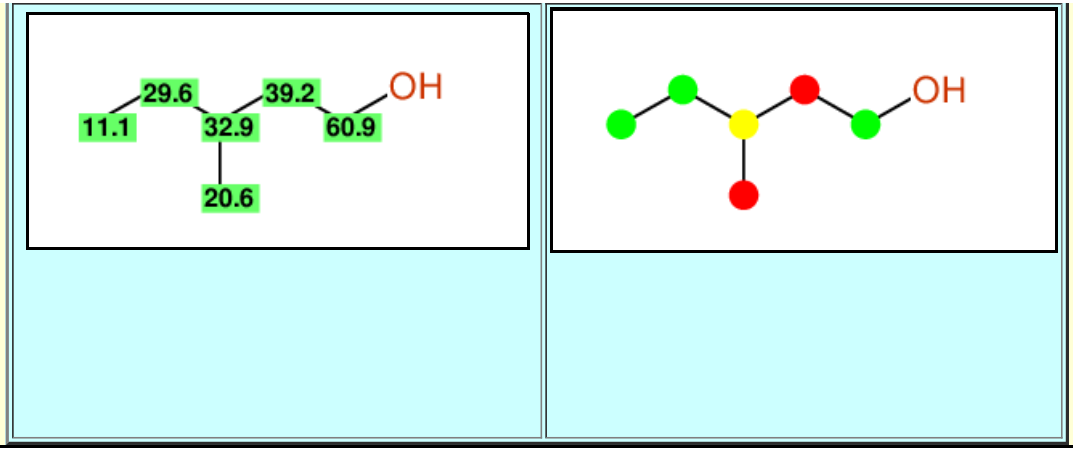
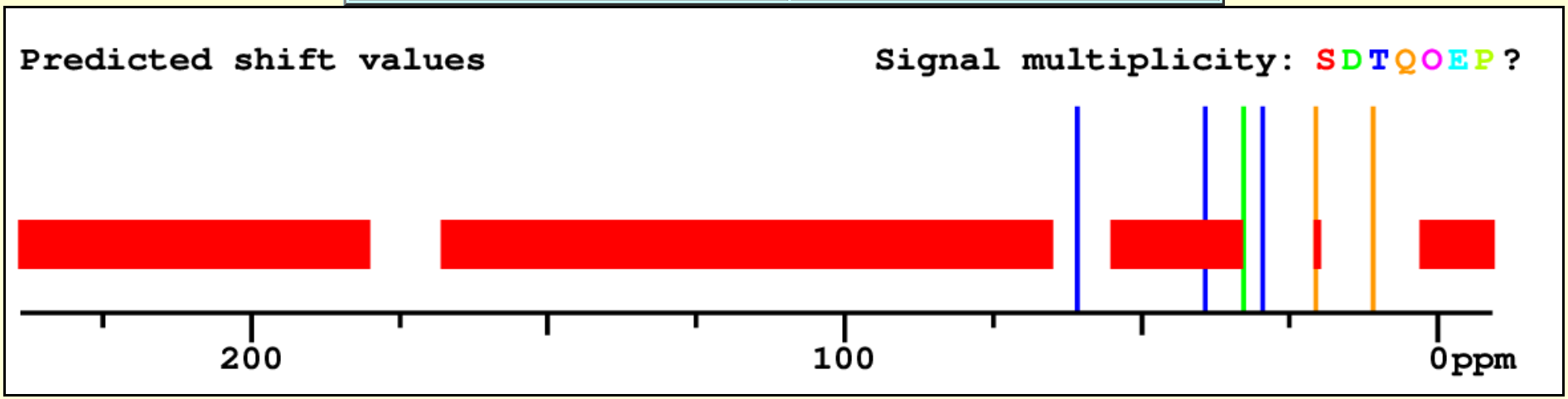
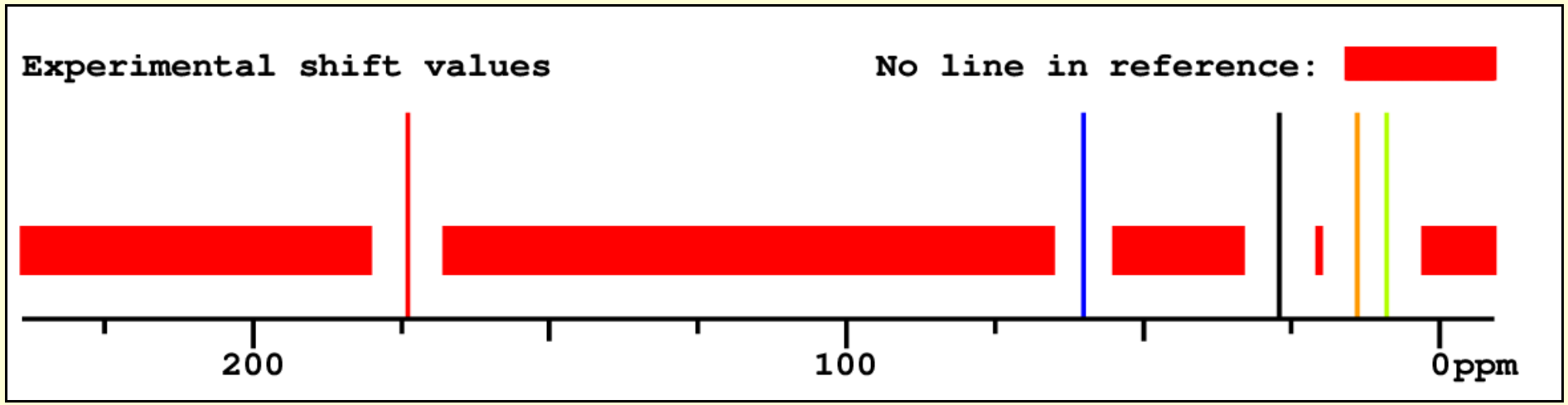
Structure Proposal #21

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


29.6
39.2
OH
11.1
32.9
60.9
20.6
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm


Experimental shift values
No line in reference:
200
100
0ppm

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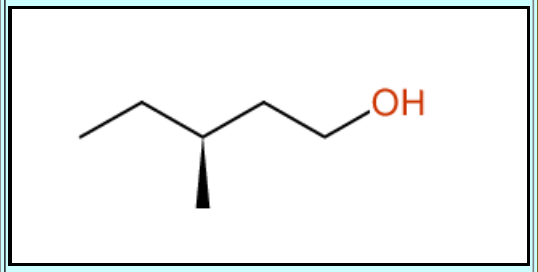
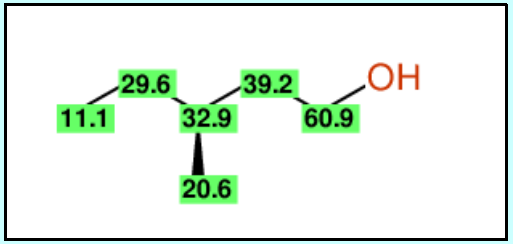
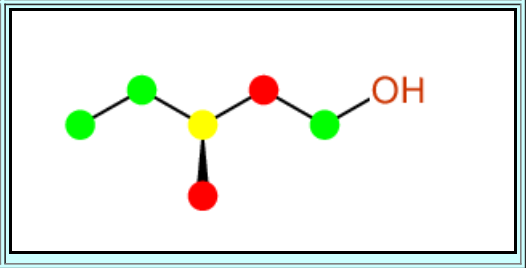
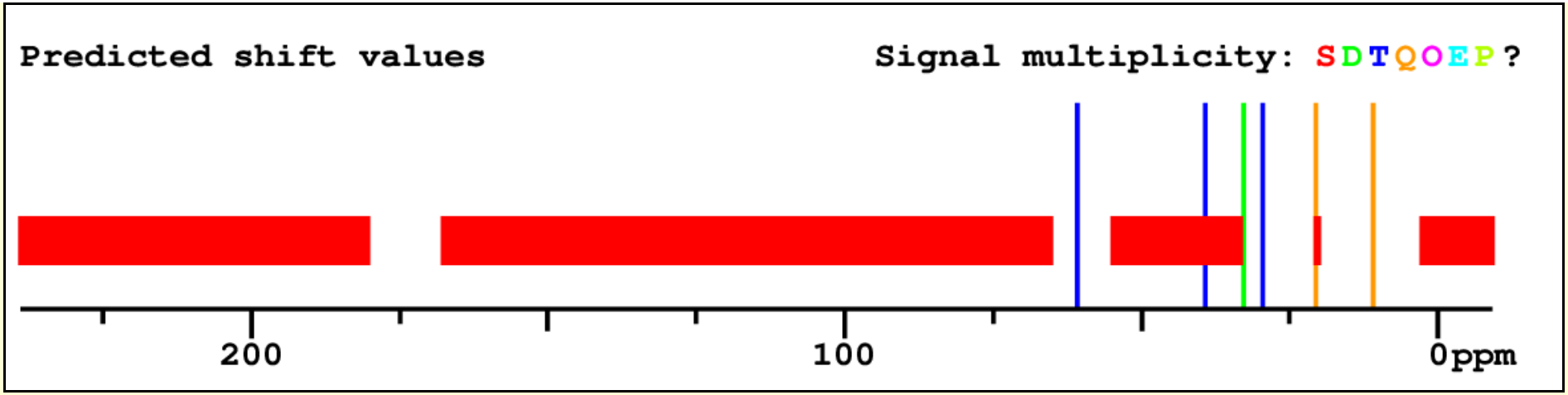
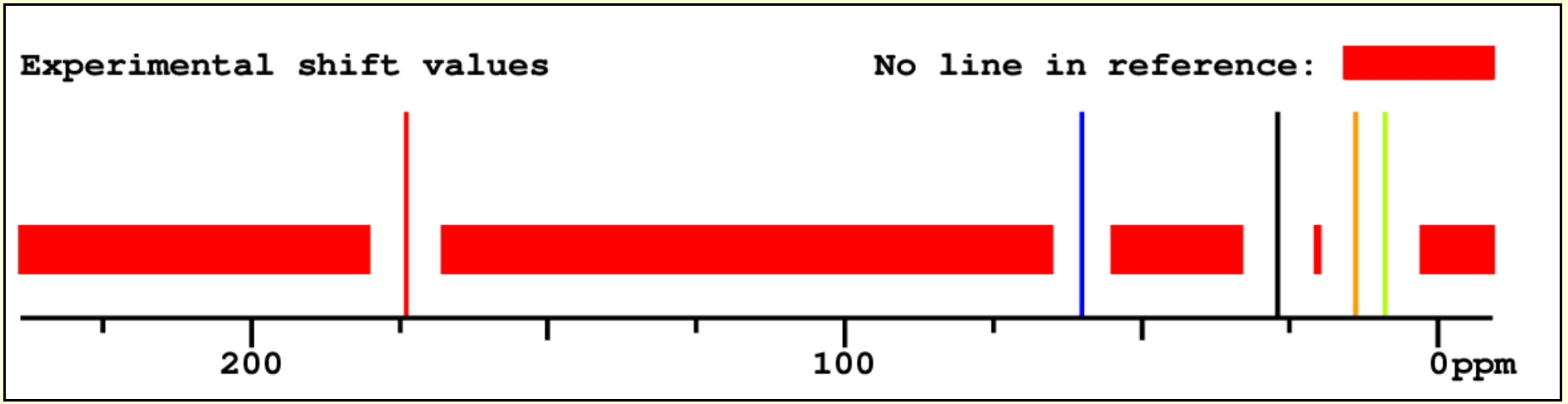
Structure Proposal #22

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





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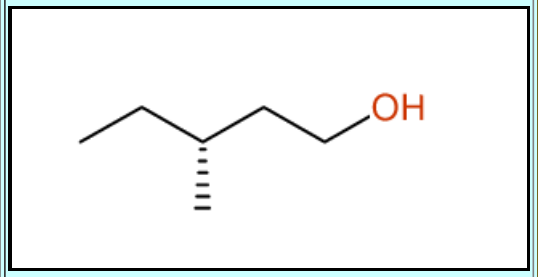
Structure Proposal #23

Structure	Similarity Measure



Deviation = 4.64 ppm
(Different pattern)

$C_6H_{14}O$

MWT = 102.07

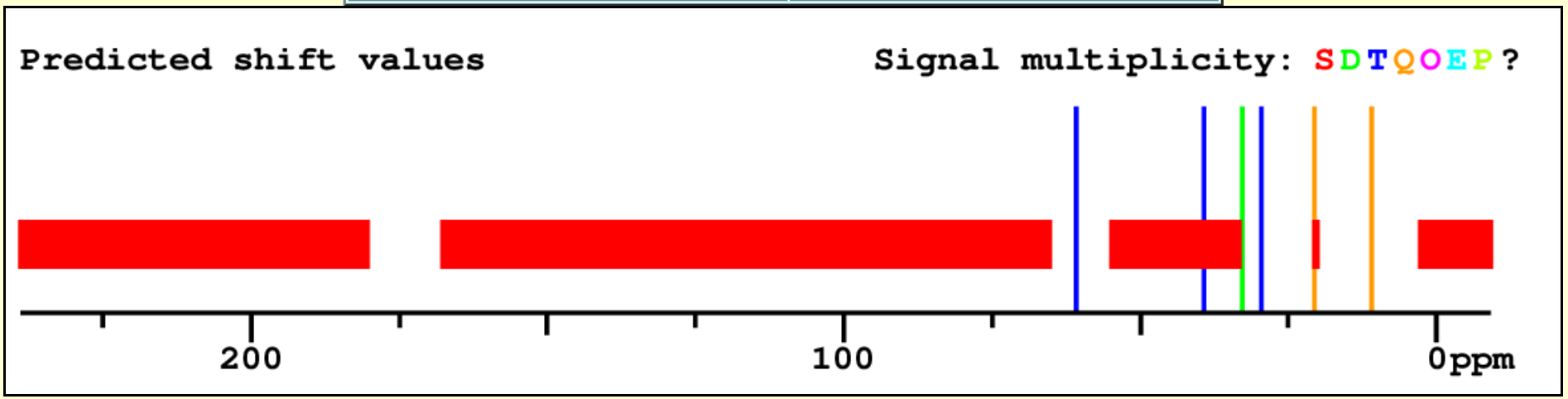
PUBCHEM

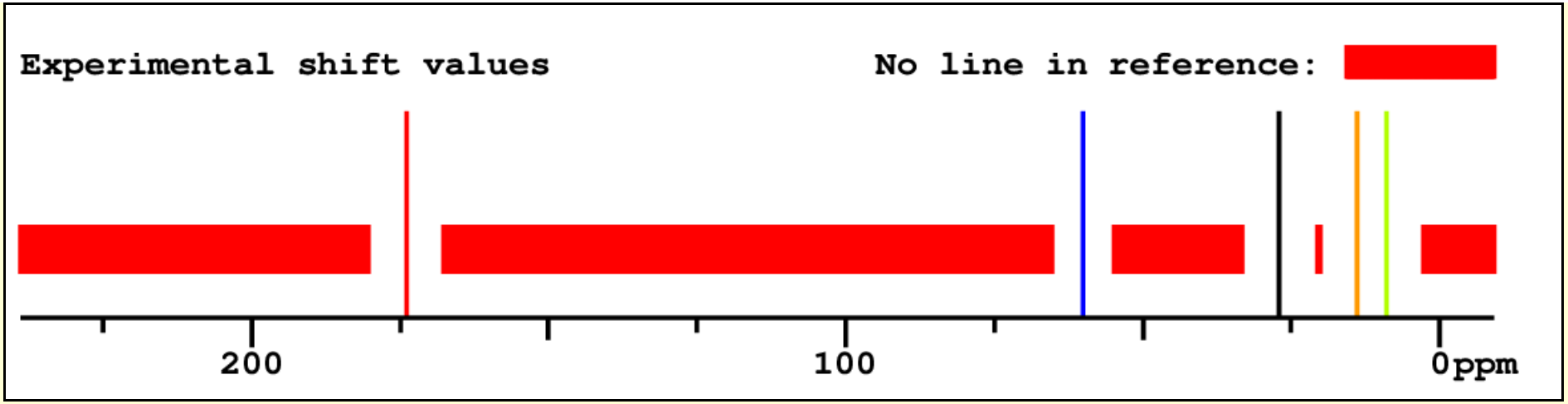
Search Web for this structure:

IWTBVKIGCDZRPL

Availability

Predicted Chemical Shiftvalues	Matching Map





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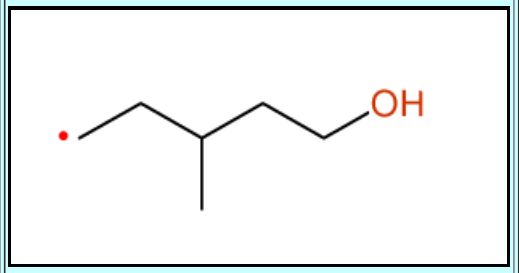
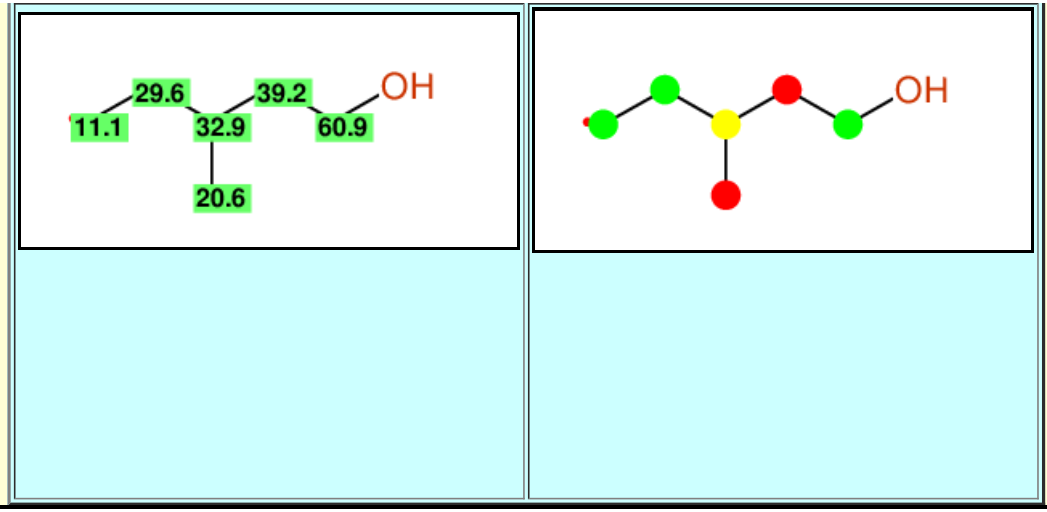
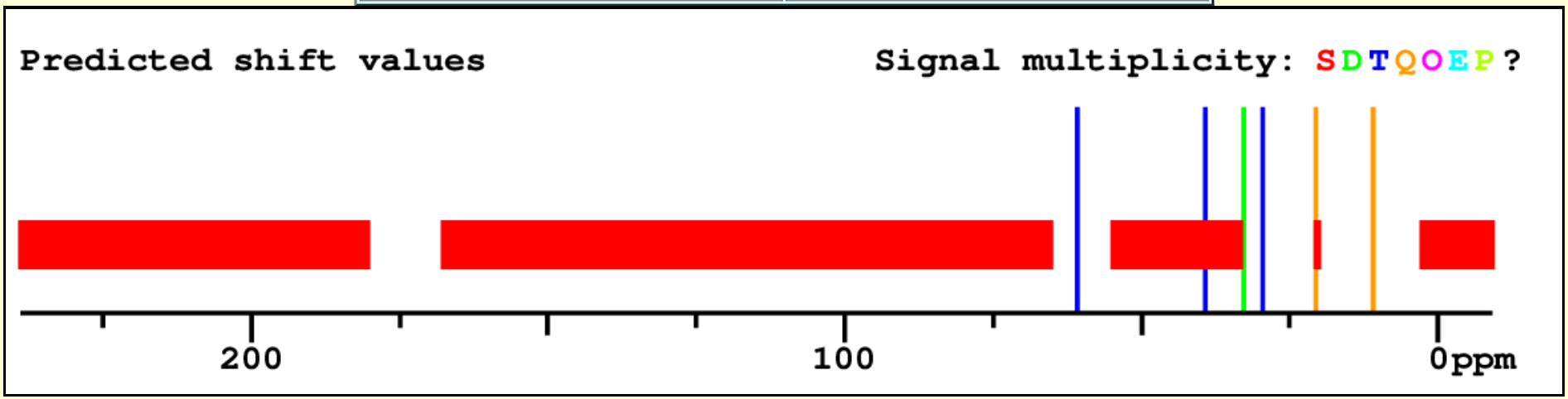
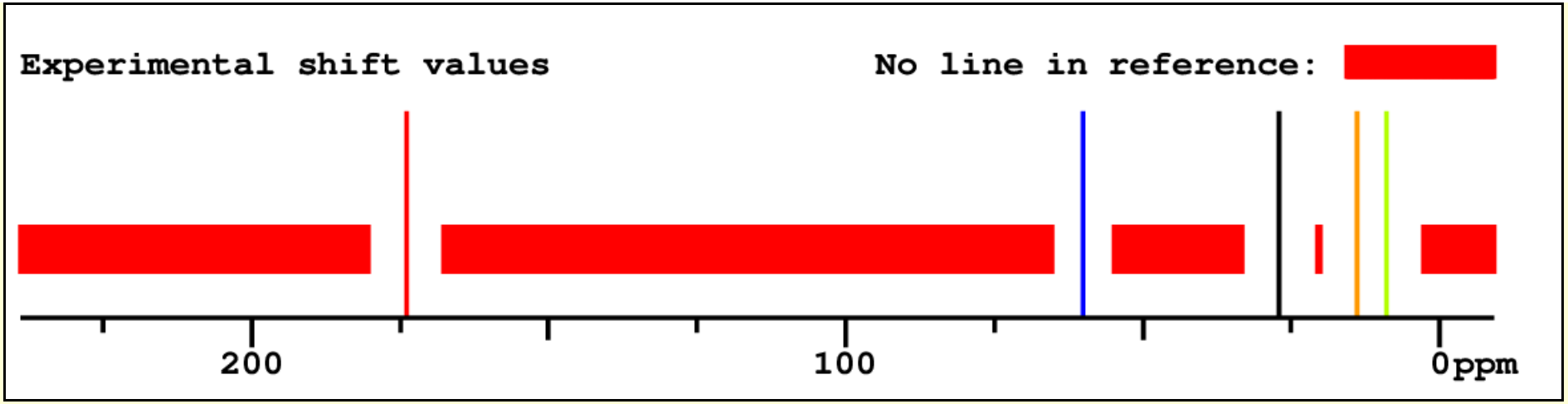
Structure Proposal #24

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


29.6
39.2
OH
11.1
32.9
60.9
20.6
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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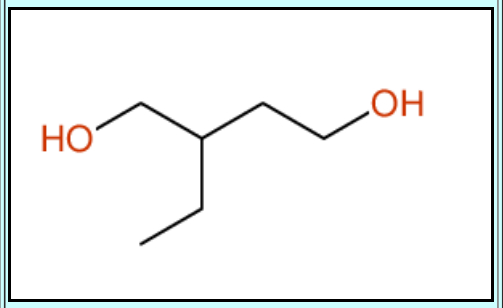
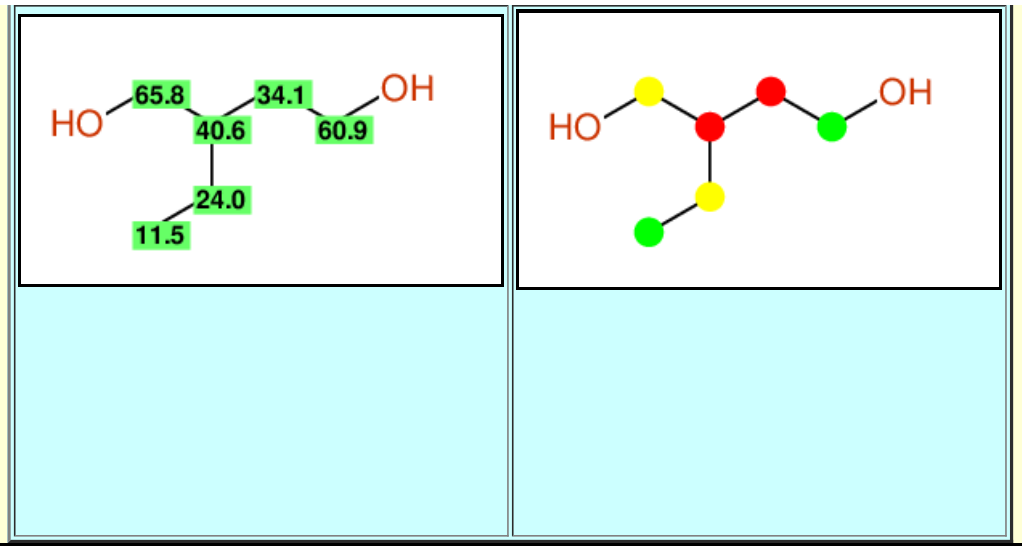
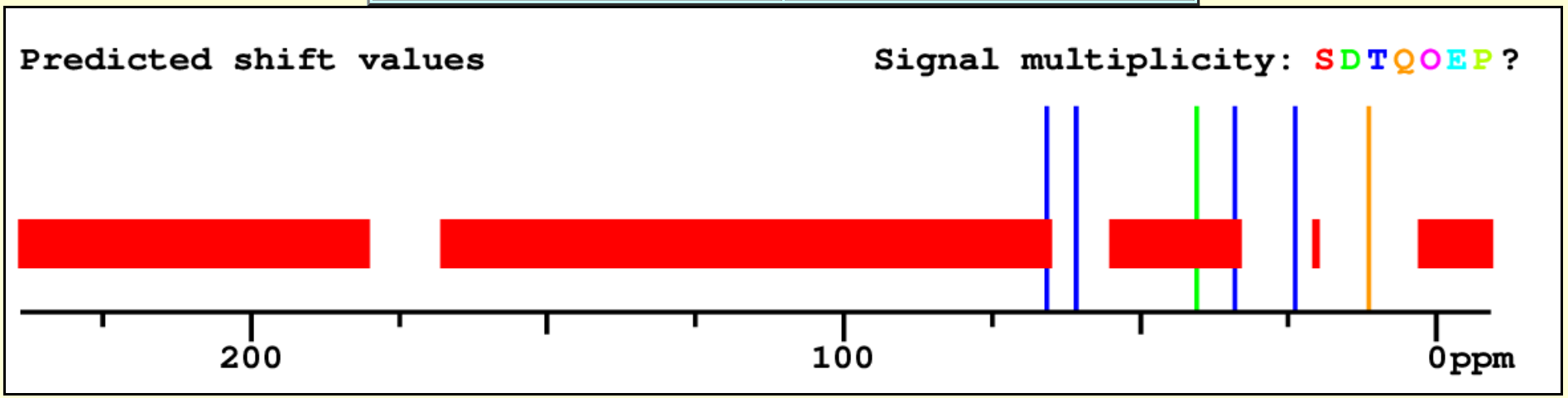
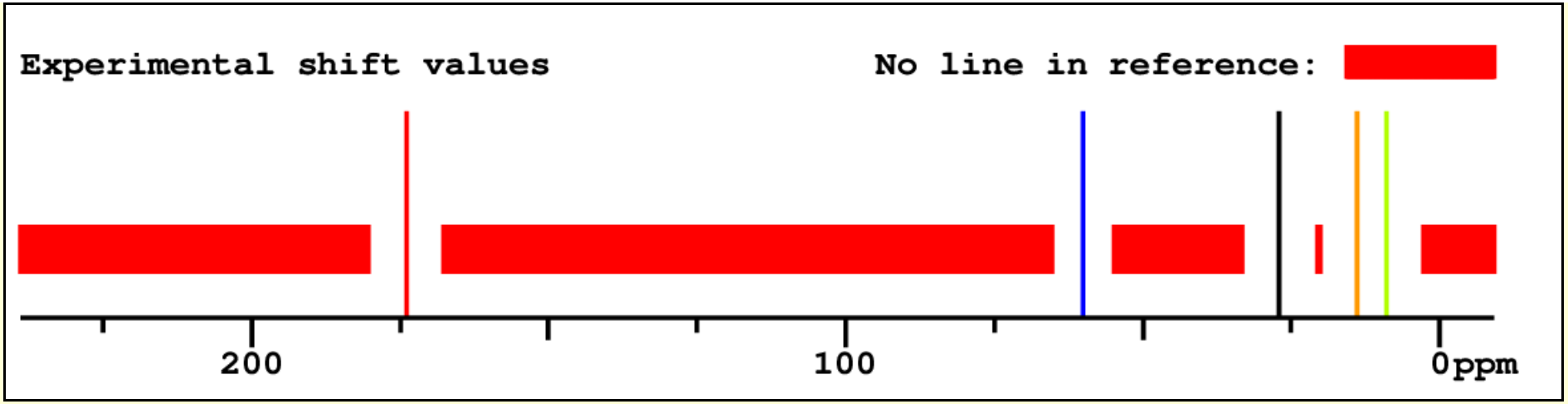
Structure Proposal #25

Structure	Similarity Measure
	**Deviation = 4.98 ppm** (Different pattern) **$C_6H_{14}O_2$** **MWT = 118.07** **PUBCHEM** **Search Web for this structure:** **CYVMBANVYOZFIG**
Predicted Chemical Shiftvalues	**Matching Map**


HO
65.8
34.1
OH
40.6
60.9
24.0
11.5
HO
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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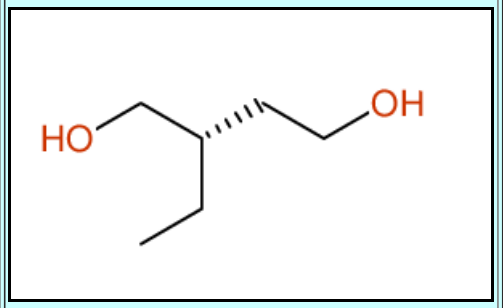
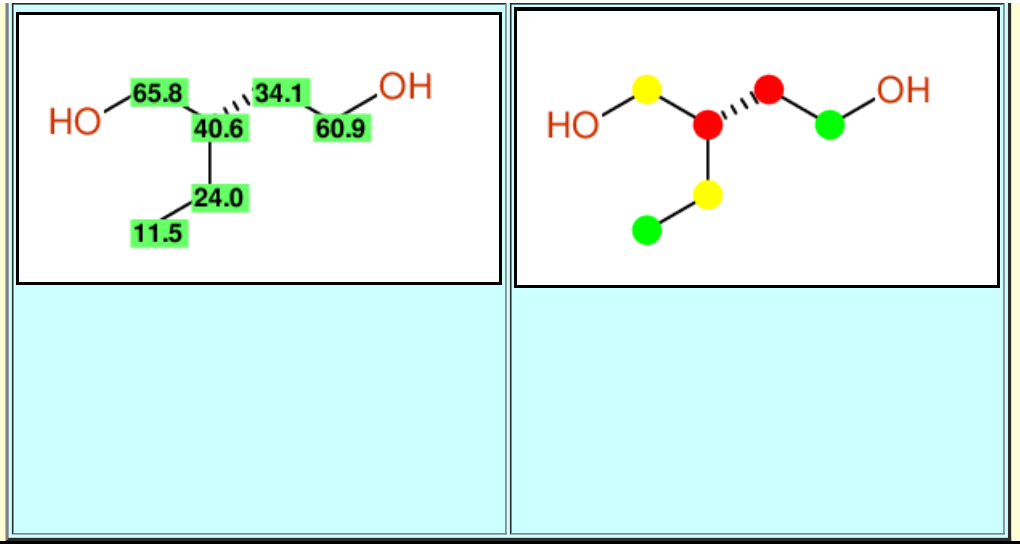
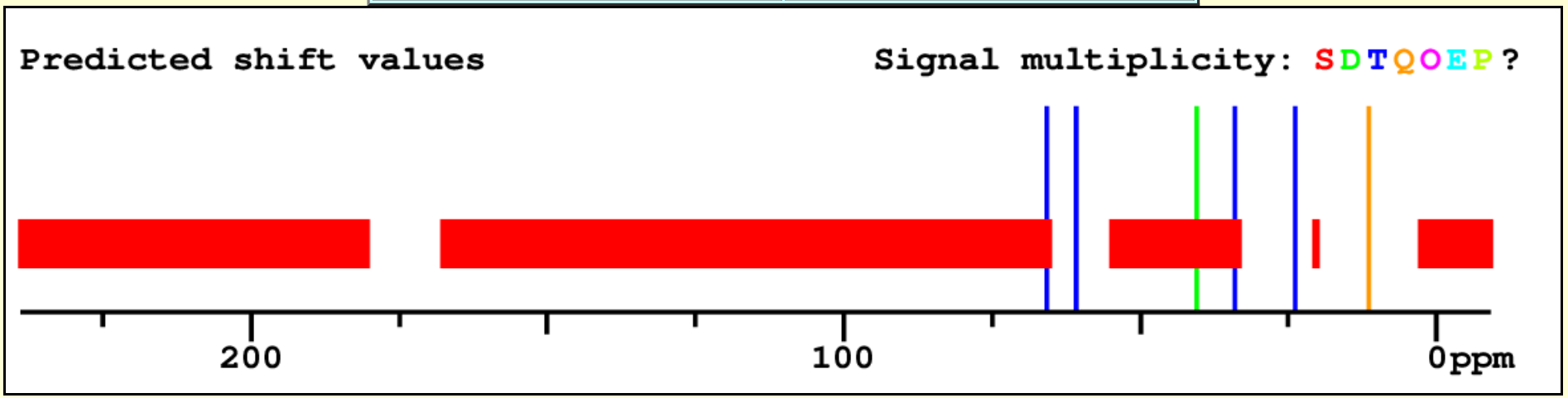
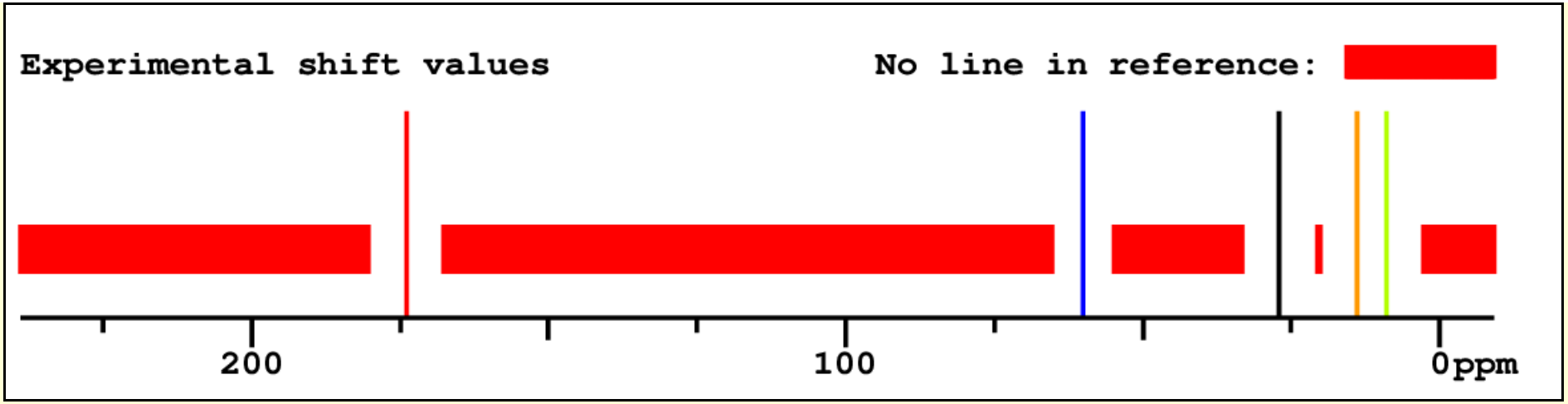
Structure Proposal #26

Structure	Similarity Measure
	**Deviation = 4.98 ppm** (Different pattern) **$C_6H_{14}O_2$** **MWT = 118.07** **PUBCHEM** **Search Web for this structure:** **CYVMBANVYOZFIG**
Predicted Chemical Shiftvalues	**Matching Map**


HO
65.8
34.1
OH
40.6
60.9
24.0
11.5
HO
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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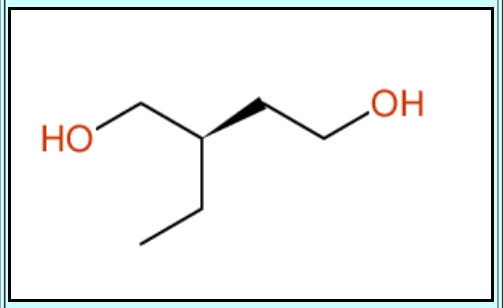
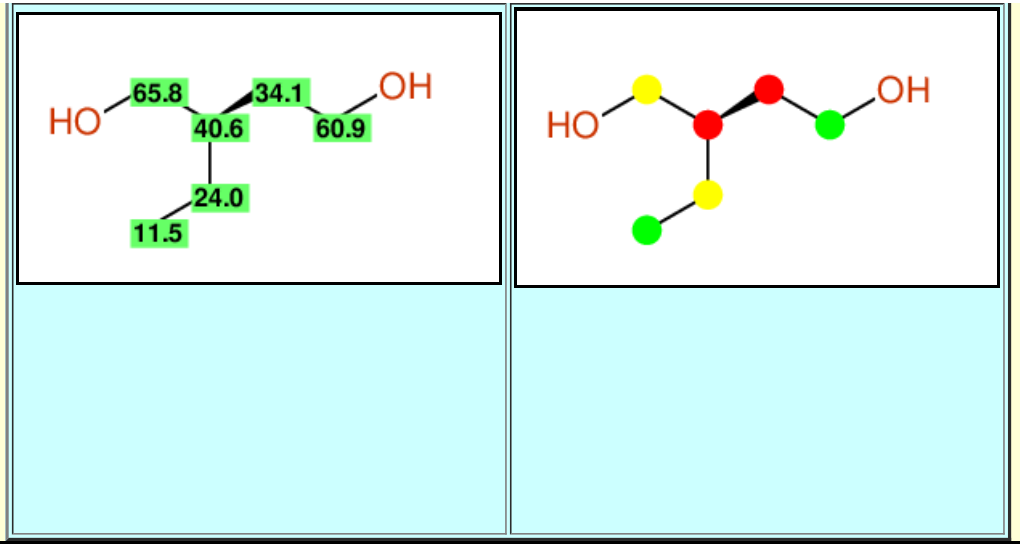
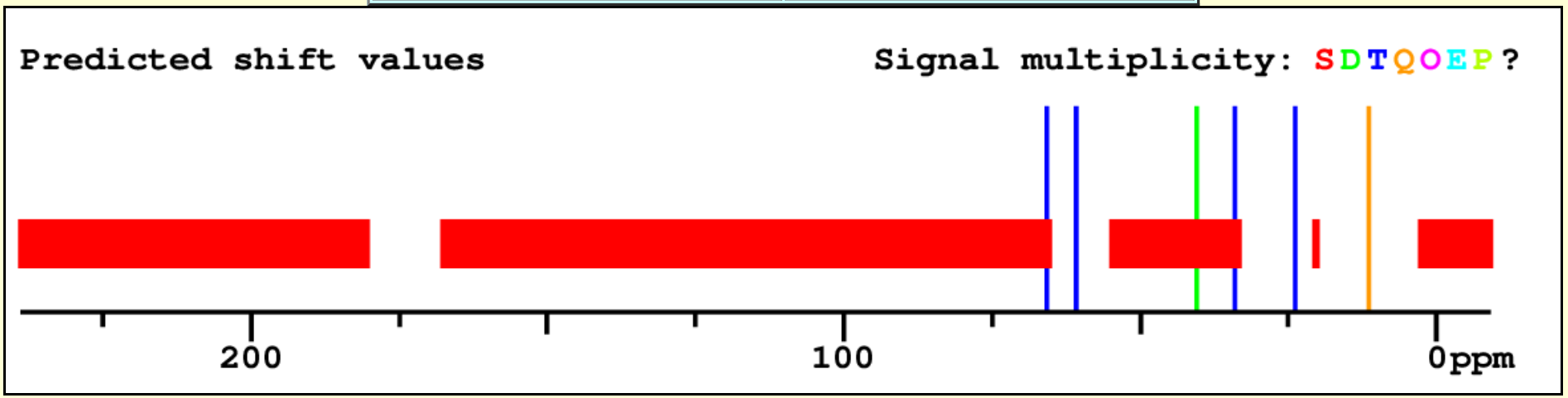
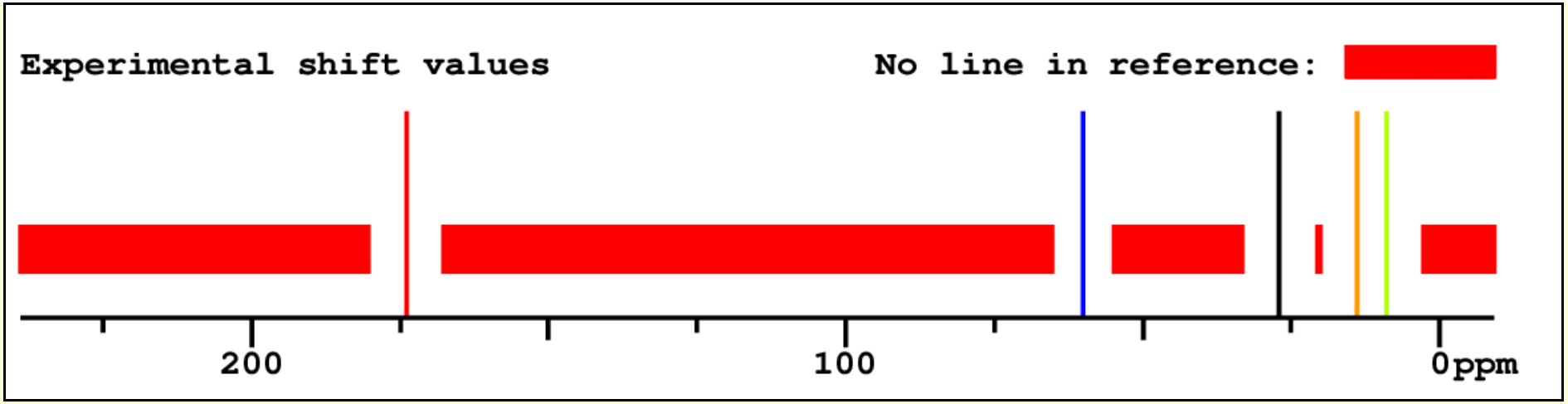
Structure Proposal #27

Structure	Similarity Measure
	**Deviation = 4.98 ppm** (Different pattern) **$C_6H_{14}O_2$** **MWT = 118.07** **PUBCHEM** **Search Web for this structure:** **CYVMBANVYOZFIG**
Predicted Chemical Shiftvalues	**Matching Map**


HO
65.8
34.1
OH
40.6
60.9
24.0
11.5
HO
OH


Predicted shift values
Signal multiplicity: SDTQOEP?
200
100
0ppm



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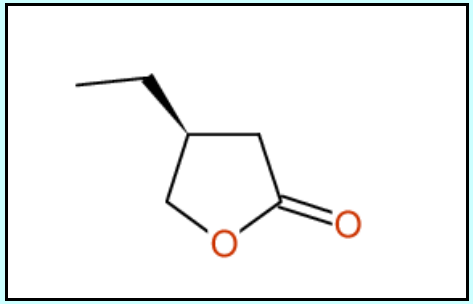
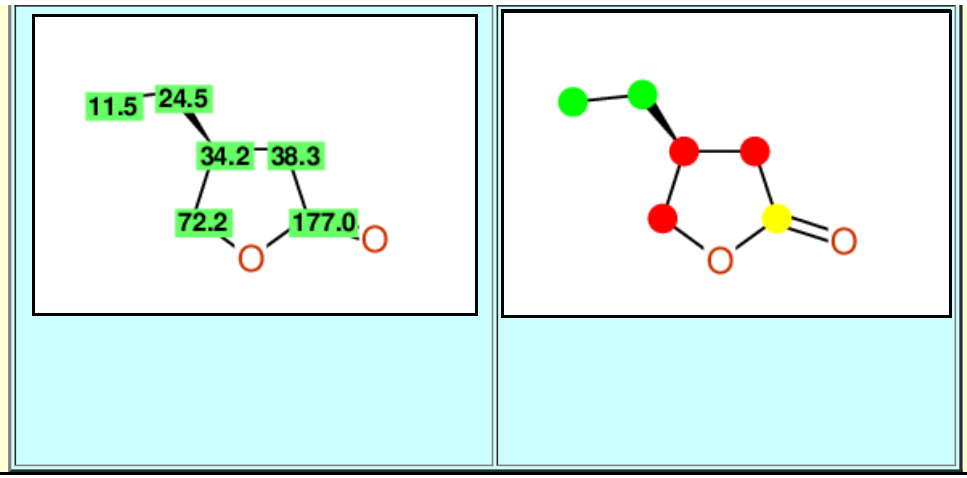
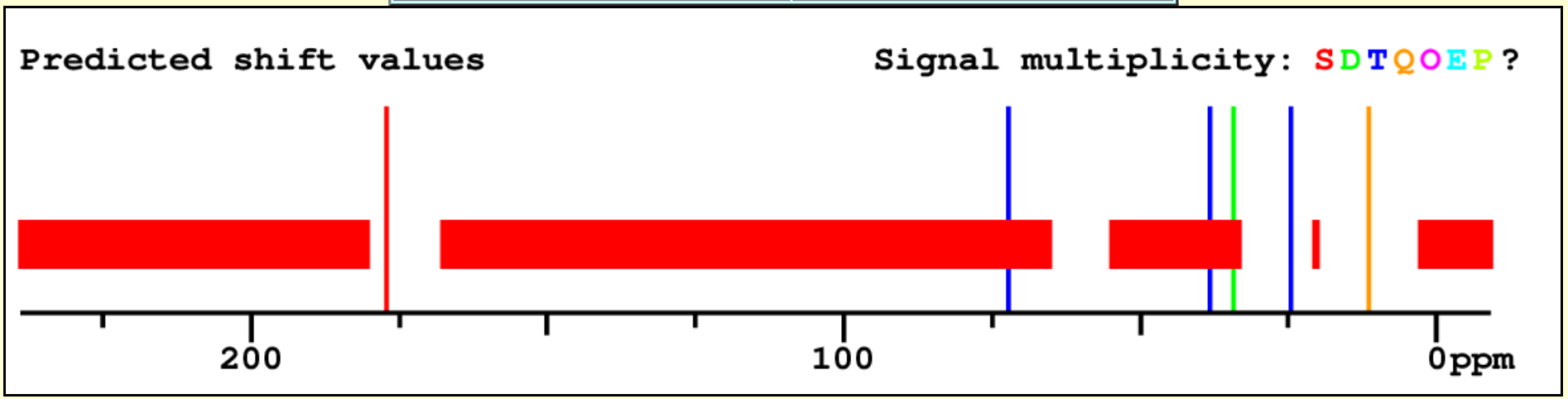
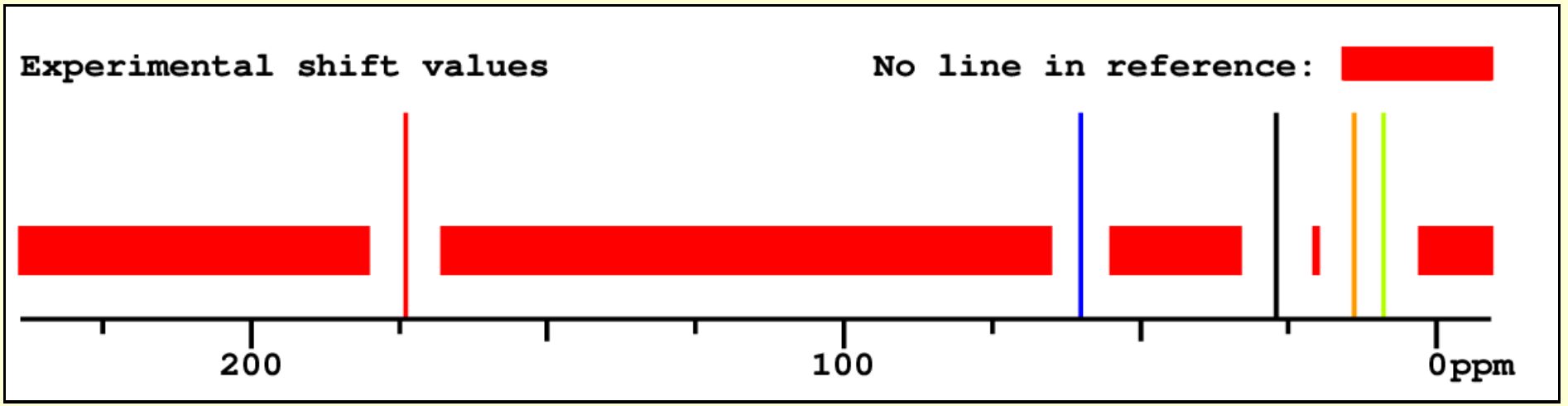
Structure Proposal #28

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


11.5
24.5
34.2
38.3
72.2
177.0
O
O
O


Predicted shift values
Signal multiplicity: SDTQQOEP?
200
100
0ppm


Experimental shift values
No line in reference:
200
100
0ppm

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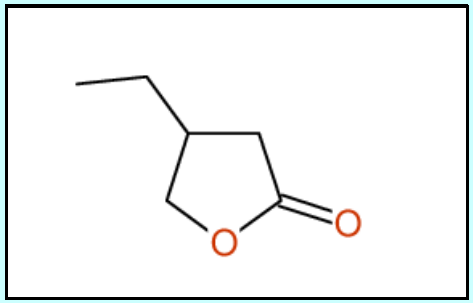
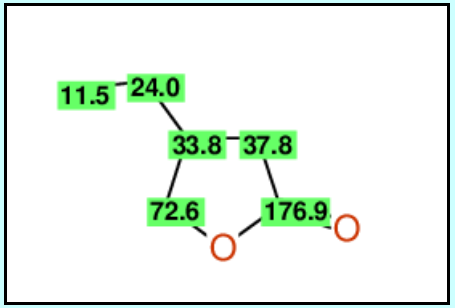
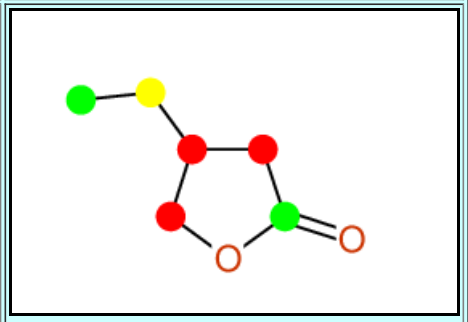
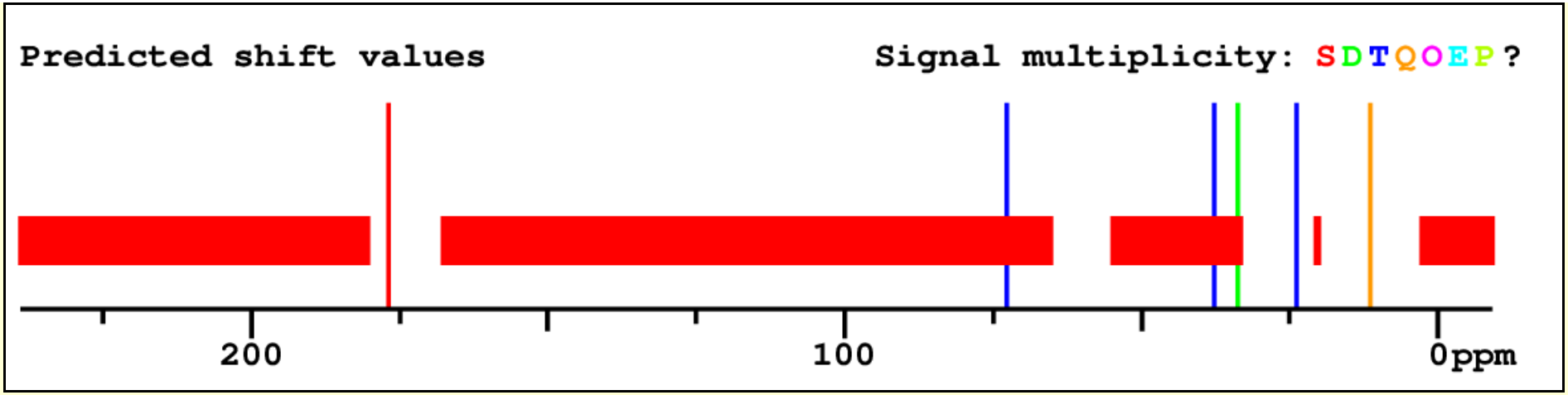
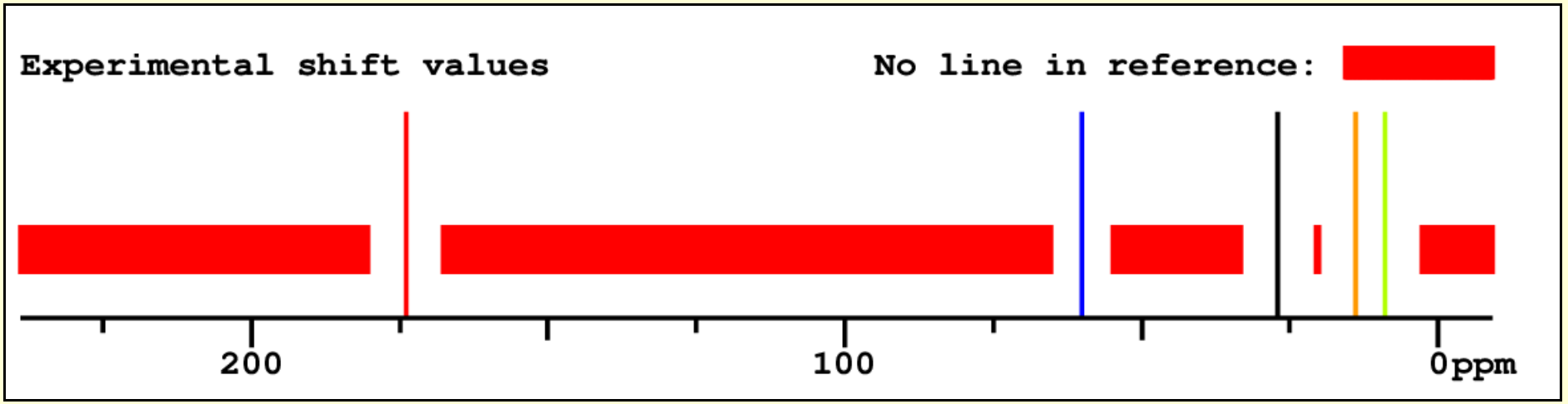
Structure Proposal #29

Structure	Similarity Measure
	**Deviation = 6.88 ppm** (Different pattern) **$C_6H_{10}O_2$** **MWT = 114.07** **PUBCHEM** **Search Web for this structure:** **MDQZVJSUBKPTHG** Availability
Predicted Chemical Shiftvalues	**Matching Map**
	





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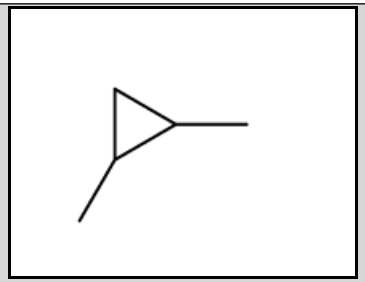
Summary of the 1 most frequently occurring parent ring systems within the 27 best-fitting entries

Occurence: 1 in 27	

Summary of Processing

Checking existence of data and counting them:	74,435,185 entries in 0.206 seconds
Applying restraints from elemental composition:	1.761 seconds, 2,773,229 entries remain
Applying restraints from number of signals:	1.946 seconds, 170,467 entries remain
Searching 1,444,403,916 chemical shift values line-per-line:	12.016 seconds
Best 1,562 entries selected for analysis:	2.543 seconds
Ranking of 1,562 entries by similarity:	0.388 seconds
Deviation of best match:	0.87 ppm
Creating table and linking 1,562 structures to 475,803 INCHIKEY-pages:	0.353 seconds
Detailled Analysis of 29 structures including graphical representation:	13.172 seconds
Analysis of 27 structures for common parent ring systems	0.004 seconds
Data transfered from disk:	406 MBytes out of 272,265 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 19:07
Page finished on 2021:05:19 at 19:08

Have a nice day !