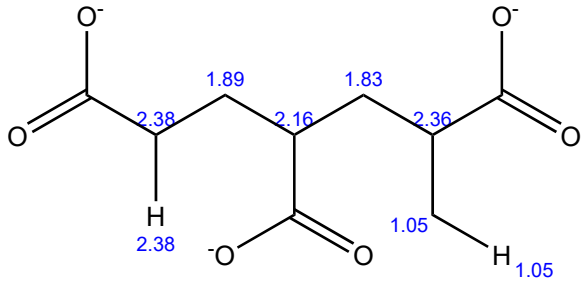
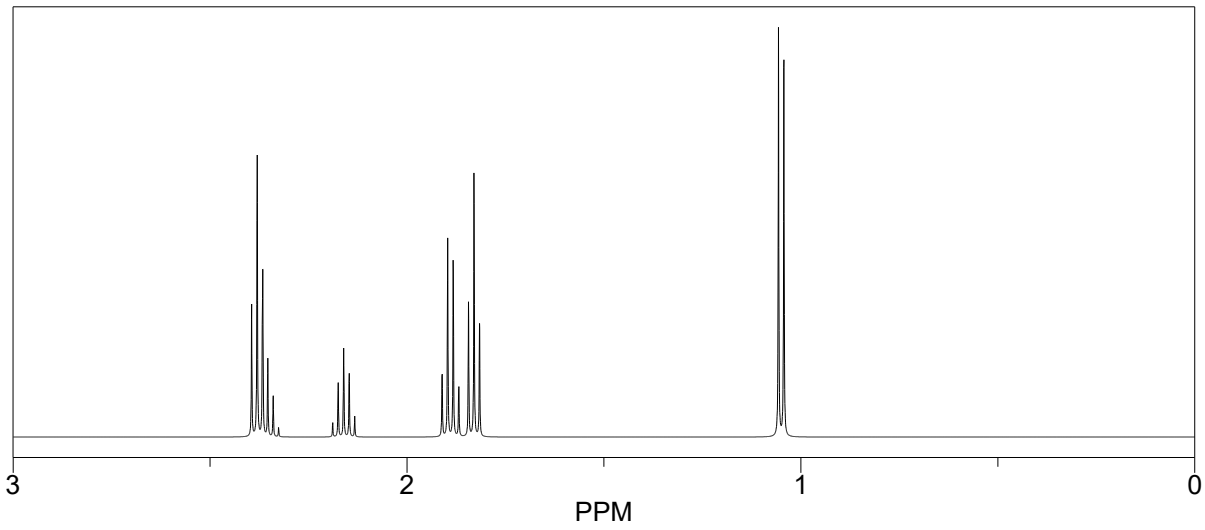
ChemNMR ^{1}H Estimation



Estimation quality is indicated by color: good, medium, rough



Protocol of the H-1 NMR Prediction (Lib=SU Solvent=DMSO 500 MHz):

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
CH	2.16	1.50	methine
		0.86	1 alpha -C=O
		-0.10	1 beta -C
		-0.10	1 beta -C
CH	2.36	1.50	methine
		0.86	1 alpha -C=O
		0.10	1 alpha -C
		-0.10	1 beta -C
CH2	2.38	1.37	methylene
		1.07	1 alpha -C=O
		-0.06	1 beta -C
CH2	1.83	1.37	methylene
		0.29	1 beta -C=O
		-0.06	1 beta -C
		0.29	1 beta -C=O
		-0.06	1 beta -C
CH2	1.89	1.37	methylene
		0.29	1 beta -C=O
		-0.06	1 beta -C
		0.29	1 beta -C=O
CH3	1.05	0.86	methyl
		0.21	1 beta -C=O
		0.05	1 beta -CC
		-0.07	general corrections
H	2.38	1.37	methylene
		1.07	1 alpha -C=O
		-0.06	1 beta -C
H	1.05	0.86	methyl
		0.21	1 beta -C=O

0.21	1 beta -C=O
0.05	1 beta -CC
-0.07	general corrections

1H NMR Coupling Constant Prediction

shift	atom index	coupling partner	constant	and vector
2.16	9			
		8	7.0	H-C-CH-H
		13	7.0	H-C-CH-H
2.36	3			
		8	7.0	H-C-CH-H
		1	6.8	H-C-CH2-H
		2	6.8	H-C-CH2-H
2.38	14			
		13	7.1	H-CH-CH-H
1.83	8			
		9	7.0	H-CH-C-H
		3	7.0	H-CH-C-H
1.89	13			
		9	7.0	H-CH-C-H
		4	7.1	H-CH-CH-H
		14	7.1	H-CH-CH-H
1.05	2			
		3	6.8	H-CH2-C-H
2.38	4			
		13	7.1	H-CH-CH-H
1.05	1			
		3	6.8	H-CH2-C-H