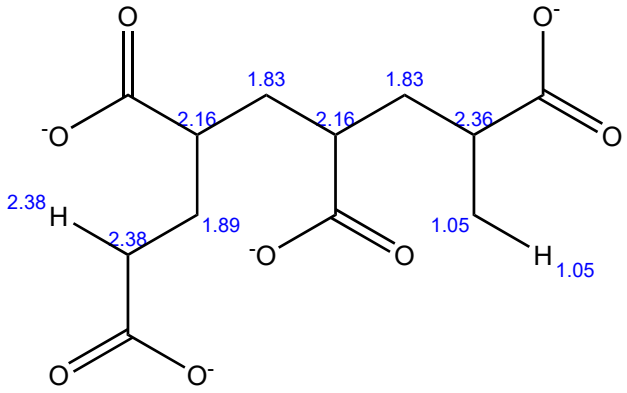
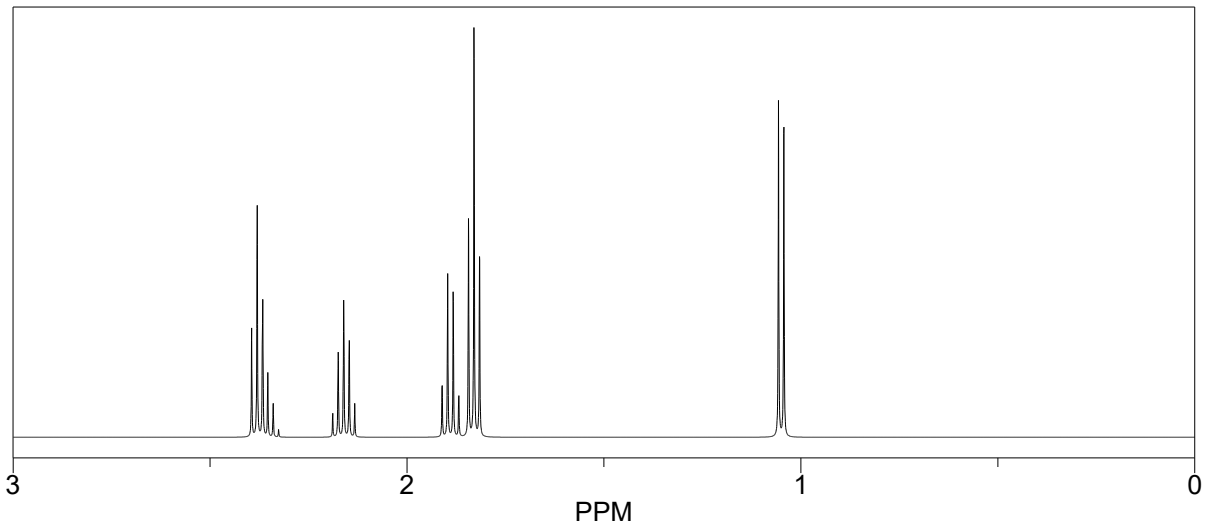
ChemNMR ^{1}H Estimation



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	2.16	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	1.83	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

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                          0.00      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
                         0.05      1 beta -CC
                        -0.07      general corrections

1H NMR Coupling Constant Prediction

shift   atom index  coupling partner, constant and vector

2.16        9
                    13   7.0  H-C-CH-H
                     8   7.0  H-C-CH-H
2.16       14
                    13   7.0  H-C-CH-H
                    18   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       19
                    18   7.1  H-CH-CH-H
1.83       13
                     9   7.0  H-CH-C-H
                    14   7.0  H-CH-C-H
1.83        8
                     9   7.0  H-CH-C-H
                     3   7.0  H-CH-C-H
1.89       18
                    14   7.0  H-CH-C-H
                     4   7.1  H-CH-CH-H
                    19   7.1  H-CH-CH-H
1.05        2
                     3   6.8  H-CH2-C-H
2.38        4
                    18   7.1  H-CH-CH-H
1.05        1
                     3   6.8  H-CH2-C-H
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