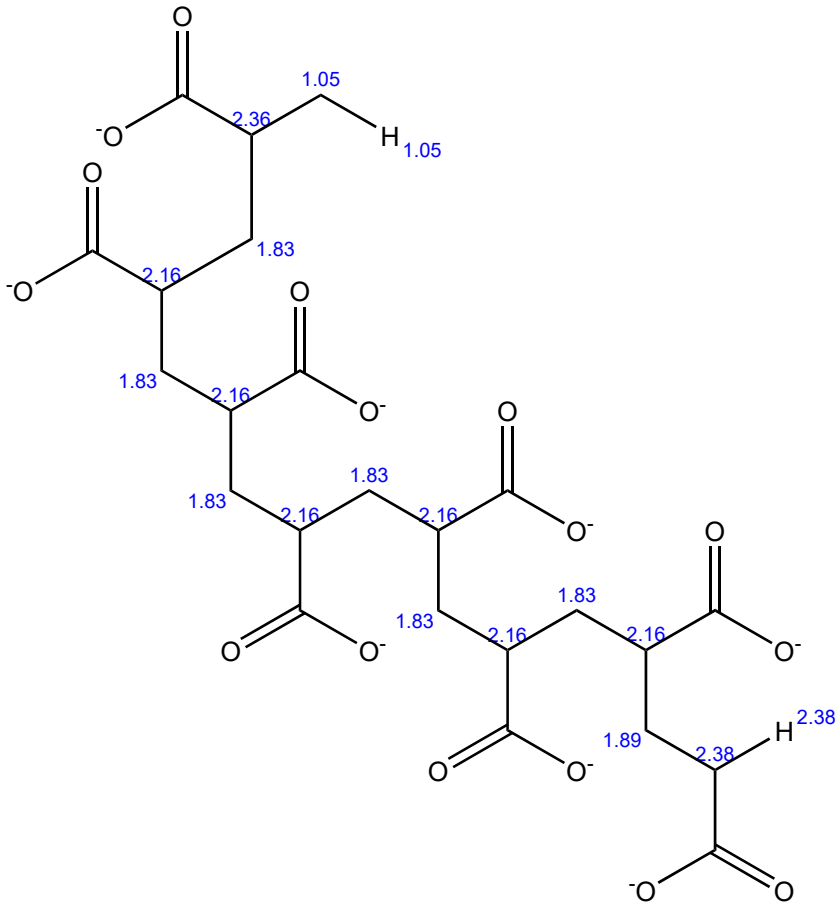
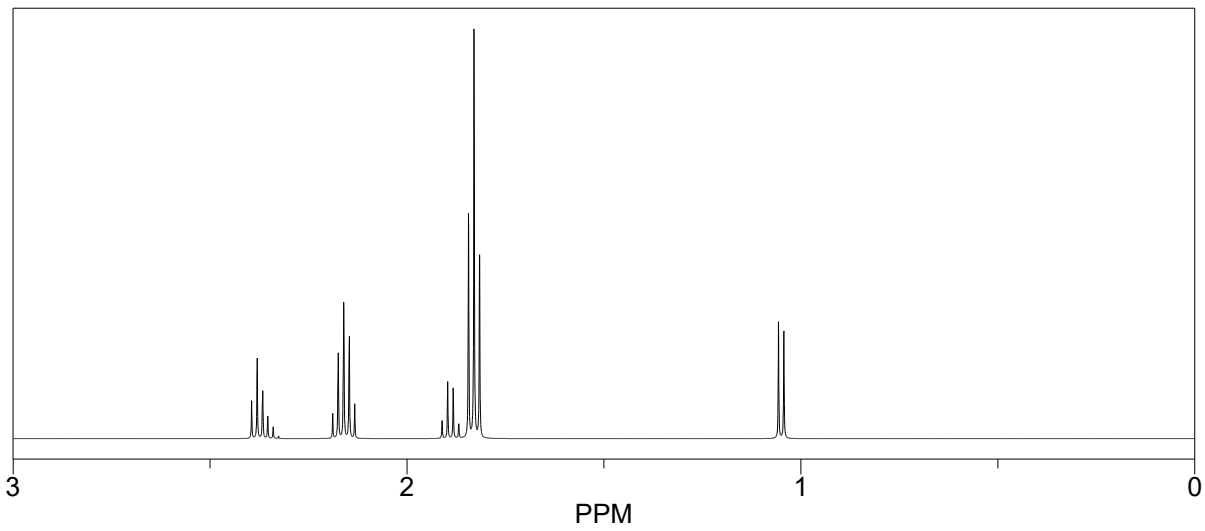
ChemNMR ^{1}H Estimation



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

```
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  2.16              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  2.16              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
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
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
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
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1H NMR Coupling Constant Prediction

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shift   atom index  coupling partner, constant and vector

2.16       19
                 23   7.0  H-C-CH-H
                 18   7.0  H-C-CH-H
2.16       24
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2.16	24			
		23	7.0	H-C-CH-H
		28	7.0	H-C-CH-H
2.16	14			
		18	7.0	H-C-CH-H
		13	7.0	H-C-CH-H
2.16	29			
		28	7.0	H-C-CH-H
		33	7.0	H-C-CH-H
2.16	9			
		13	7.0	H-C-CH-H
		8	7.0	H-C-CH-H
2.16	34			
		33	7.0	H-C-CH-H
		38	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	39			
		38	7.1	H-CH-CH-H
1.83	23			
		19	7.0	H-CH-C-H
		24	7.0	H-CH-C-H
1.83	18			
		19	7.0	H-CH-C-H
		14	7.0	H-CH-C-H
1.83	28			
		24	7.0	H-CH-C-H
		29	7.0	H-CH-C-H
1.83	13			
		14	7.0	H-CH-C-H
		9	7.0	H-CH-C-H
1.83	33			
		29	7.0	H-CH-C-H
		34	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	38			
		34	7.0	H-CH-C-H
		4	7.1	H-CH-CH-H
		39	7.1	H-CH-CH-H
1.05	2			
		3	6.8	H-CH2-C-H
2.38	4			
		38	7.1	H-CH-CH-H
1.05	1			
		3	6.8	H-CH2-C-H