

¹³C-NMR SPECTROSCOPY OF FATTY ACIDS AND DERIVATIVES

Esters of Glycerol and Other Polyhydric Alcohols

Monoacylglycerols (MAG) and diacylglycerols (DAG) are important emulsifying agents. They are also used in acetylated forms. Acylated derivatives of other polyhydric alcohols such as carbohydrates, propane-1,2-diol, trimethylolpropane, and pentaerythritol are also useful compounds. Chemical shifts for many of these compounds have been reported.

- There are five different classes of glycerol esters (see [Table 1](#)) and chemical shifts associated with the glycerol carbon are useful for both qualitative and quantitative purposes, especially the glyc-2 signals. Values for glyc-2 lie between 68 and 75 ppm and those for glyc-1 and 3 are between 61 and 66 ppm. In “symmetrical” molecules (2-MAG, 1,3-DAG, and TAG) the signals for glyc-1 and glyc-3 are the same. They differ in the “unsymmetrical” molecules. These chemical shifts can be used to analyse mixtures of glycerol esters (Gunstone) and the results of a ring test have been reported (Grone). Signals for C1 and C2 in the acyl chains also differ between the various glycerol esters, but these are less useful (Gunstone).
- Chemical shifts for acetylated monoacylglycerols are listed in [Table 2](#).
- Chemical shifts for acylated derivatives of propane-1,2-diol are given in [Table 3](#).
- Chemical shifts for fully acylated derivatives of trimethylolpropane, and pentaerythritol are given in [Table 4](#).
- Sugar esters: chemical shifts are recorded for sucrose-6'-O-mono esters (10:0, 12:0, 14:0, 16:0, and 18:0) and sucrose-6-O-mono esters (12:0, 14:0, 16:0, and 18:0). Full details are given in the original paper (Sarney *et al.*).

Table 1. Chemical shifts (ppm) for glycerol carbon atoms in monoacylglycerols (mag), diacylglycerols (dag), and triacylglycerols (tag) based on palmitic and oleic acids (Vlahov).

	Palmitic			Oleic		
	Glyc-1	Glyc-2	Glyc-3	Glyc-1	Glyc-2	Glyc-3
1-mag	63.34	70.26	65.11	63.35	70.26	65.13
2-mag*	61.9	74.9	61.9			
1,2-dag	61.54	72.11	62.02	61.56	72.12	62.00
1,3-dag	65.04	68.38	65.04	65.03	68.34	65.03
tag	62.10	68.87	62.10	62.08	68.87	62.08

* values taken from Gunstone, fatty acid not indicated.

Table 2. Chemical shifts (ppm) for glycerol and other carbon atoms in acetylated monoacylglycerols (Gunstone).
Compounds 1-4 are the 1-monoacylglycerol (1), its 2-acetate (2), 3-acetate (3), and 2,3-diacetate (4).

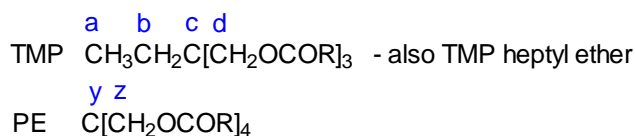
	1	2	3	4
Glyc-1	65.15	62.07	65.00	62.00
Glyc-2	70.26	72.39	68.14	69.16
Glyc-3	63.39	61.40	65.26	62.33
C1	174.31	173.84	173.96	173.38
COCH₃ (α)	-	-	20.79	20.69
			171.10	170.57
COCH₃ (β)	-	21.00	-	20.88
		170.98		170.16

Table 3. Chemical shifts (ppm) for mono and di-esters of propane-1,2-diol (Gunstone).

	C1	C2	C3	P1	P2	P3
1-ester	173.99	34.23	24.99	69.46	66.13	19.2
2-ester	173.99	34.58	25.04	65.92	71.77	16.25
1,2-diester	173.51	34.51	25.03	65.42	67.98	16.5
	173.24	34.19	24.97			

Table 4. Chemical shifts (ppm) for fully acylated derivatives of trimethylolpropane (TMP), and pentaerythritol (PE) (Black).

	a	b	c	d	C1	y	z	C1
C₂						41.98	62.43	170.25
C₆						42.24	62.28	172.79
C₇						42.12	62.23	172.99
C₈	7.48	23.36	41.01	63.72	172.71	42.17	62.26	172.95
C₉	7.47	23.38	40.92	63.76	172.73	42.25	62.27	172.81
C₁₀	7.42	23.31	40.89	63.75	172.96	42.18	62.27	172.88
C₁₂	7.39	23.33	40.87	63.82	173.26	42.11	62.28	173.11
C₇ ether	7.77	23.29	43.22	71.49	71.28			



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