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ELECTRONICAL SUPLEMENTARY MATERIALS

for

Synthesis, characterization and reactivity of the six-membered cyclic glycerol carbonate bearing free hydroxyl group

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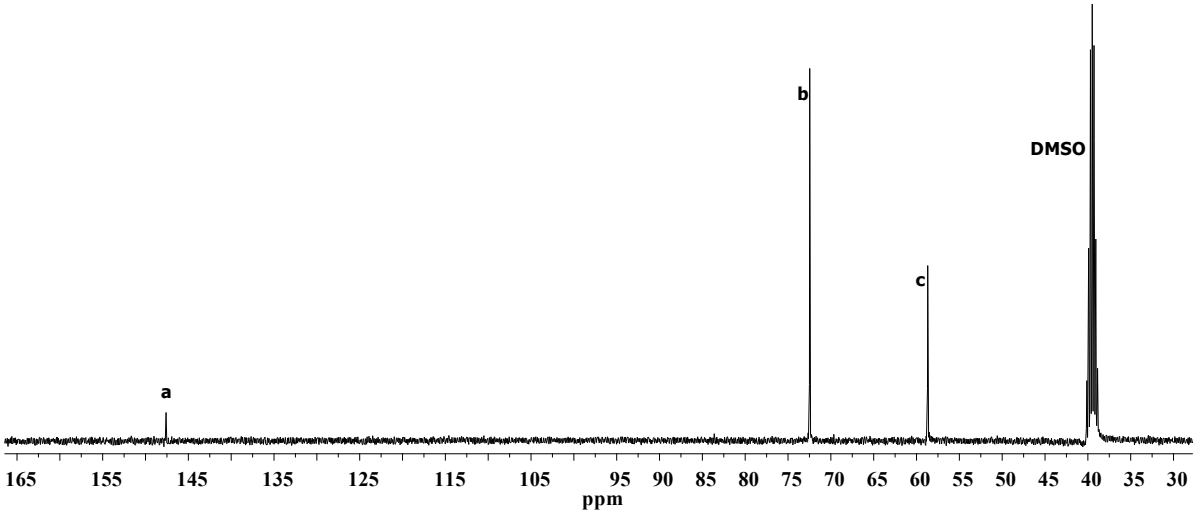

Figure 1S. ^{13}C NMR (400 MHz, DMSO-d_6) spectrum of 5-hydroxy-1,3-dioxan-2-one (**2**).

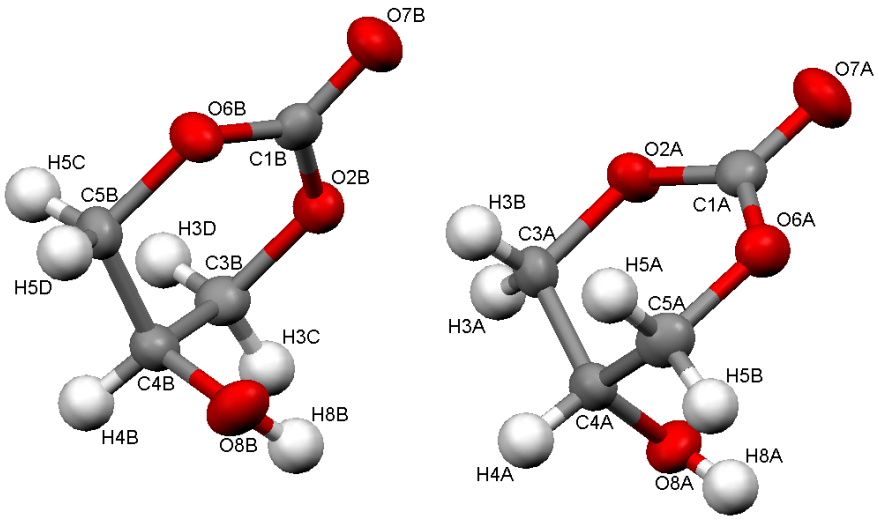

Figure 2s. X-Ray structure of 5-hydroxy-1,3-dioxane-2-one (**2**). [in colour]

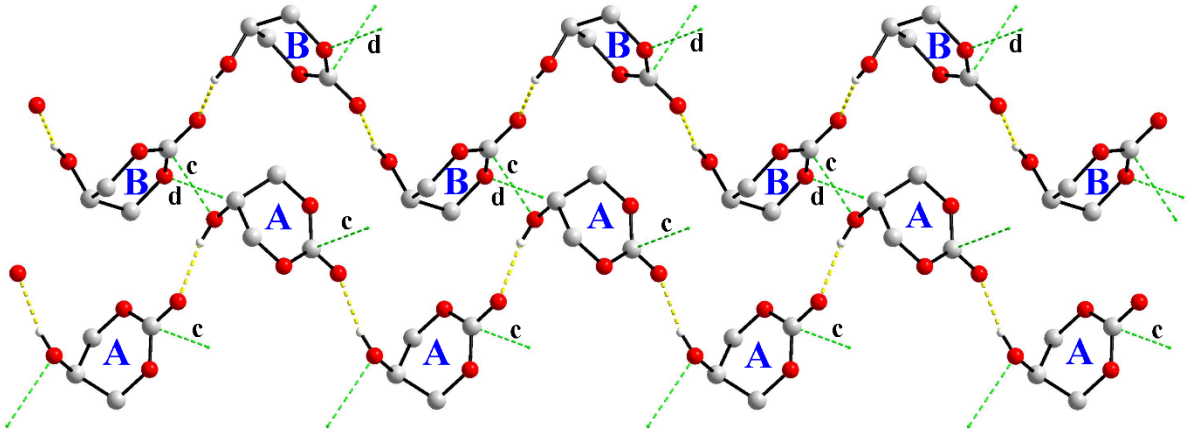

Figure 3s. Hydrogen bonded chains of two types of 5-hydroxy-1,3-dioxane-2-one (**2**) molecules. [in colour]

Table 1S. Crystal data and structure refinement for 5-hydroxy-1,3-dioxan-2-one (**2**).

Identification code	pw_cw	
Chemical formula	$C_4H_6O_4$	
Formula weight	118.09	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal size	0.60 x 0.35 x 0.25 mm	
Crystal habit	colorless prism	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.6016(4) Å	α = 90°
	b = 9.5305(4) Å	β = 119.312°
	c = 10.7702(5) Å	γ = 90°
Volume	948.88(8) $Å^3$	
Z	8	
Density (calculated)	1.653 g/cm^3	
Absorption coefficient	0.152 mm^{-1}	
F(000)	496	

Diffractometer	KM4CCD κ-axis
Radiation source	graphite-monochromated MoK_α
Theta range for data collection	3.05 to 28.61 deg
Index ranges	-14<=h<=14, -12<=k<=12, -14<=l<=14
Reflections collected / unique	16237 / 2327 [R(int) = 0.0098]
Completeness to theta = 28.00	99.0%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.96 and 0.92
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2327 / 0 / 191
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0270, wR2 = 0.0747
R indices (all data)	R1 = 0.0294, wR2 = 0.0756
Largest diff. peak and hole	0.316 and -0.278 $eÅ^{-3}$

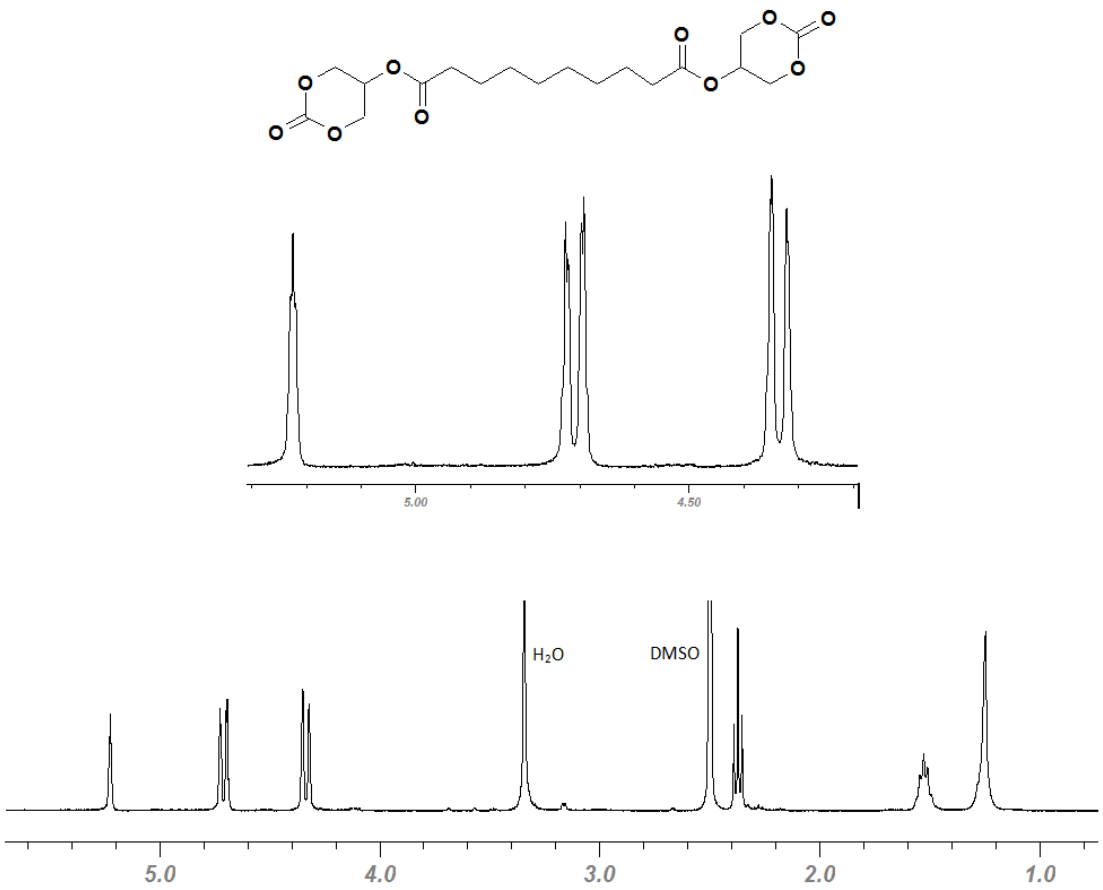

Figure 4S. ^{1}H NMR (DMSO-$d_{6,}$ 400 MHz) spectrum of of bis(2-oxo-1,3-dioxan-5-yl) sebacate (**3**); ^{1}H NMR (DMSO-$d_{6,}$ 400 MHz); δ (ppm) = 5.25-5.20 (m, 2H, C<u>H</u>O), 4.76-4.66 (m, 4H, C<u>H</u>$_{2\ cycl.}$), 4.39-4.29 (m, 4H, C<u>H</u>$_{2\ cycl.}$), 2.37 (t, 4H, COC<u>H</u>$_2$, J=7.3Hz), 1.58-1.48 (m, 4H, C<u>H</u>$_{2\ lin.}$), 1.25 (bs, 8H, C<u>H</u>$_{2\ lin.}$); ^{13}C NMR ($CDCl_{3,}$ 400 MHz); δ (ppm) = 172.9 (<u>C</u>=O$_{ester}$), (147.2 (<u>C</u>=O$_{cycl.}$), 69.8 (O<u>C</u>H$_{2cycl.}$), 62.2 (<u>C</u>HO$_{cycl.}$), 33.9 (<u>C</u>H$_2$), 28.8 (<u>C</u>H$_2$), 28.7 (<u>C</u>H$_2$), 24.6 (<u>C</u>H$_2$).

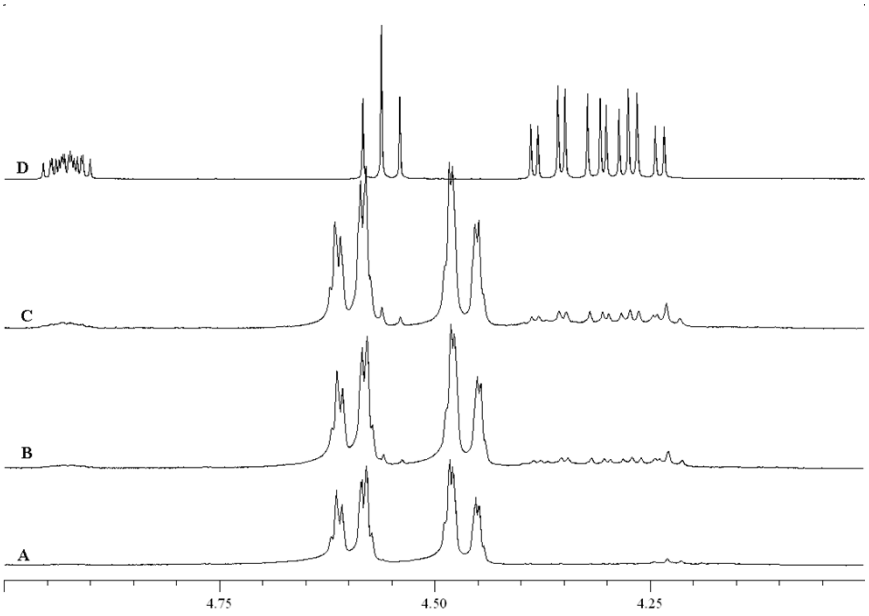

Figure 5S. Progress of isomerization of bis(2-oxo-1,3-dioxan-5-yl) sebacate (**3**) to bis[(2-oxo-1,3-dioxolan-4-yl)methyl] sebacate (**4**) monitored by ^{1}H NMR (400 MHz, DMSO-d_6). A – D reaction times: A – 0 min, B – 8 min, C – 12 min, D – 25 min.

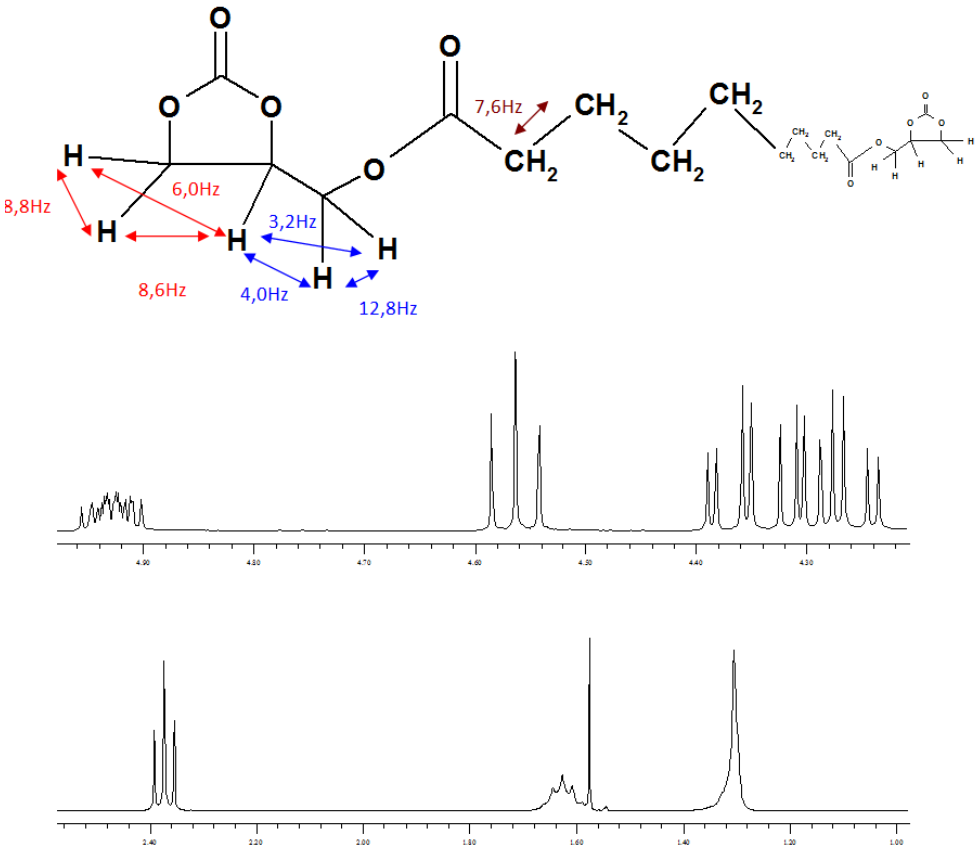

Figure 6S. ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of bis[(2-oxo-1,3-dioxolan-4-yl)methyl] sebacate (**4**); ^{1}H NMR ($CDCl_3$, 400 MHz); δ (ppm) = 4.96-4.90 (m, 2H, $CH_2\underline{H}CH_2$), 4.56 (dd, 2H, $OC\underline{H}_{2cyc.}$, J_1=8.8Hz, J_2=8.6Hz), 4.37 (dd, 2H, $OC\underline{H}_{2lin.}$, J_1= 12.8Hz, J_2=3.2Hz), 4.30 (dd, 2H, $OC\underline{H}_{2cyc.}$, J_1=8.8Hz, J_2=6.0Hz), 4.25 (dd, 2H, $OC\underline{H}_{2lin.}$, J_1=12.8Hz, J_2=4.0Hz), 2.37 (t, 4H, $COC\underline{H}_2$, J=7.6Hz), 1.68-1.58 (m, 4H, $COCH_2C\underline{H}_2$), 1.30 (bs, 8H, $COCH_2CH_2C\underline{H}_2$ $C\underline{H}_2$).