

ELECTRONICAL SUPPLEMENTARY MATERIALS

for

Novel high reactive bifunctional five- and six-membered bicyclic dicarbonate – synthesis and characterisation

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Table 1S. Crystal data and structure refinement for α,β -diglycerol dicarbonate, 56BCC

Identification code	MTAS_MON1	
Chemical formula	C ₈ H ₁₀ O ₇	
Formula weight	218.16	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.199 x 0.281 x 0.298 mm	
Crystal habit	colorless prism	
Crystal system	Monoclinic	
Space group	P1 21/c 1	
Unit cell dimensions	a = 10.5437(12) Å	$\alpha = 90^\circ$
	b = 8.0245(9) Å	$\beta = 93.598(2)^\circ$
	c = 10.8487(12) Å	$\gamma = 90^\circ$
Volume	916.08(18) Å ³	
Z	4	
Density (calculated)	1.582 g/cm ³	
Absorption coefficient	1.246 mm ⁻¹	
F(000)	456	

Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS	
Radiation source	INCOATEC I μ S micro-focus source, CuK α	
Theta range for data collection	6.87 to 67.46 deg	
Index ranges	-12 ≤ h ≤ 12, -9 ≤ k ≤ 9, -12 ≤ l ≤ 12	
Reflections collected / unique	10146 / 1641 [R(int) = 0.0251]	
Completeness to theta = 28.00	99.6%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7900 and 0.7080	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1641 / 49 / 194	
Goodness-of-fit on F ²	1.193	
Final R indices [I > 2 σ (I)]	R1 = 0.0332, wR2 = 0.0844	
R indices (all data)	R1 = 0.0340, wR2 = 0.0851	
Largest diff. peak and hole	0.284 and -0.182 eÅ ⁻³	
R.M.S. deviation from mean	0.039 eÅ ⁻³	

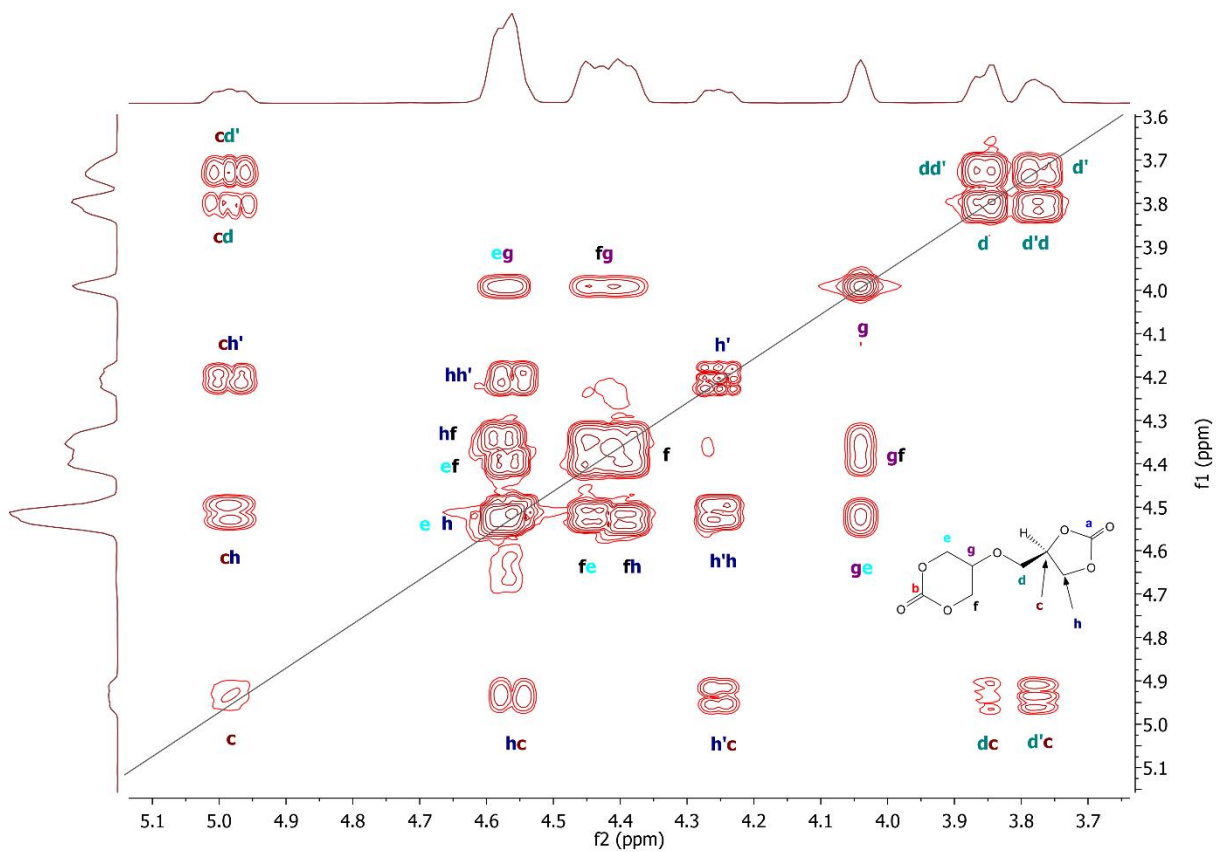


Figure 1S ^1H - ^1H COSY of 56BCC

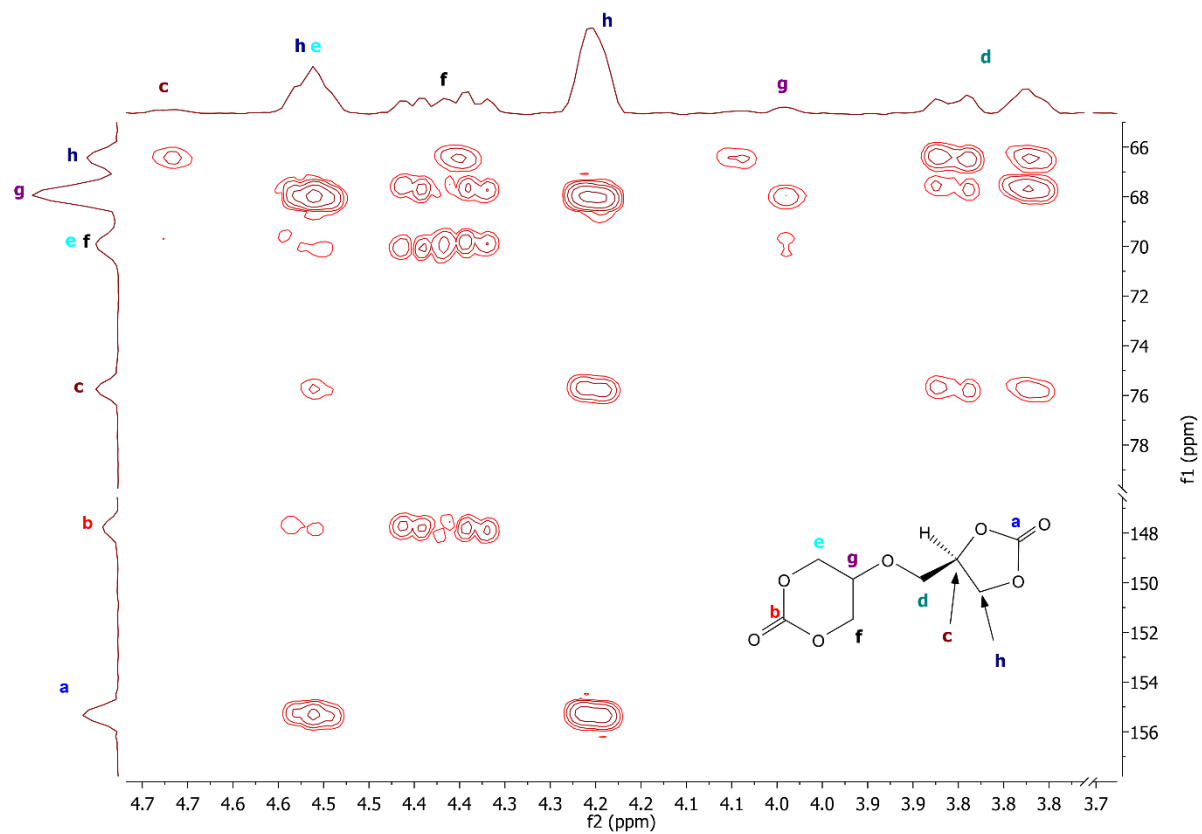


Figure 2S ^1H - ^{13}C HMBC of 56BCC

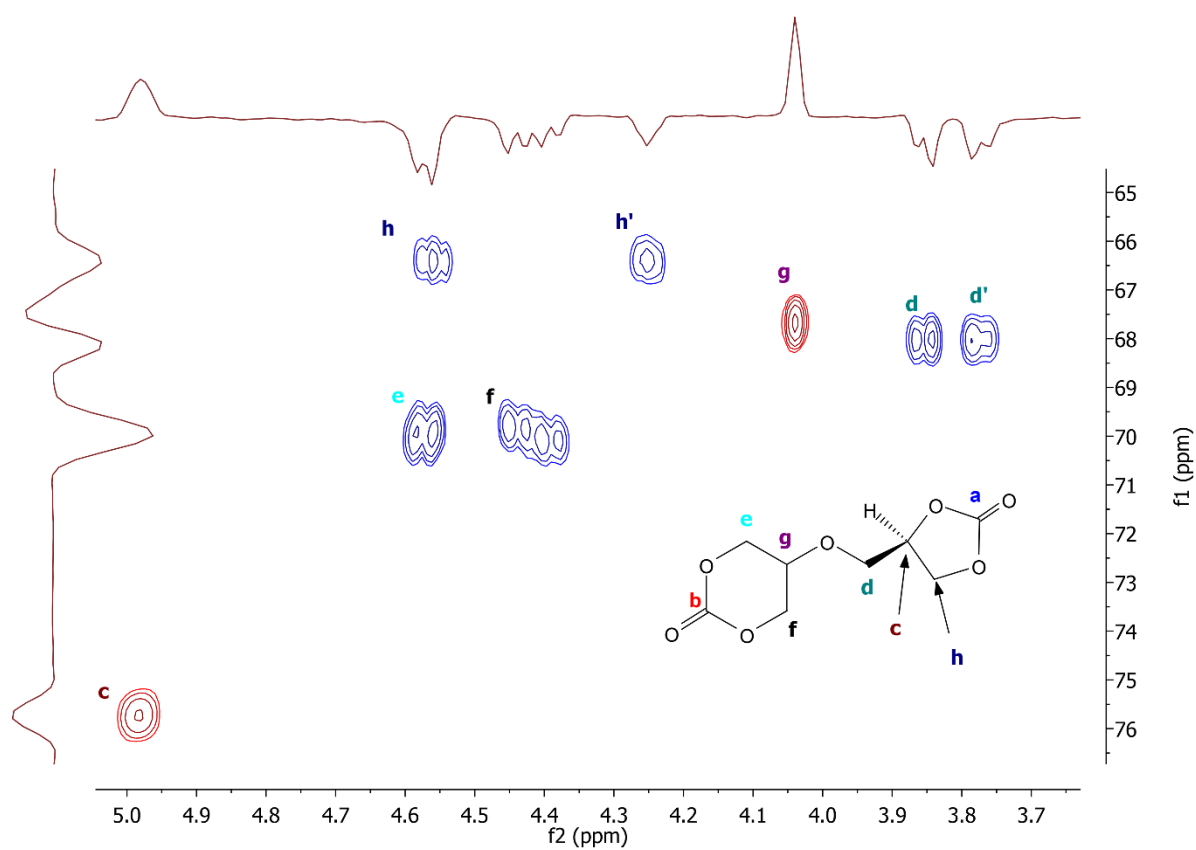


Figure 3S ^1H - ^{13}C HMQSC of 56BCC

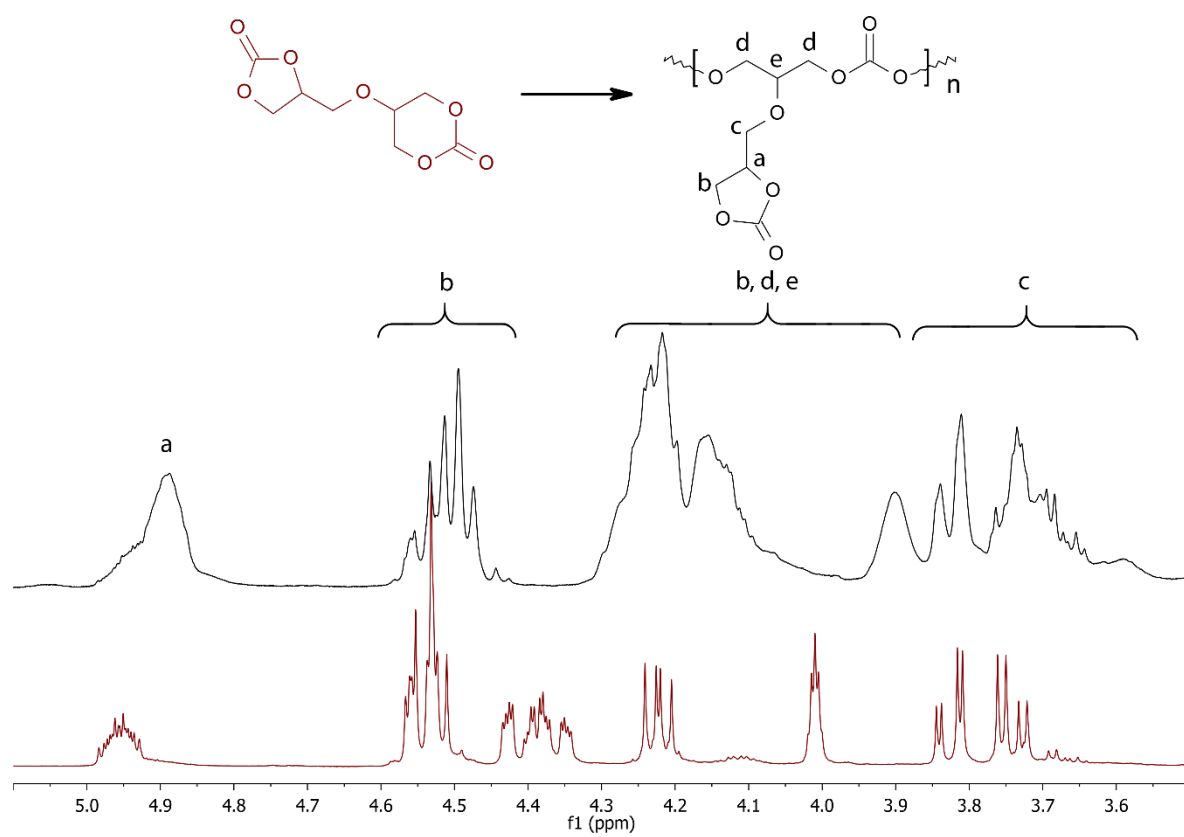


Figure 4S ^1H NMR of polycarbonate

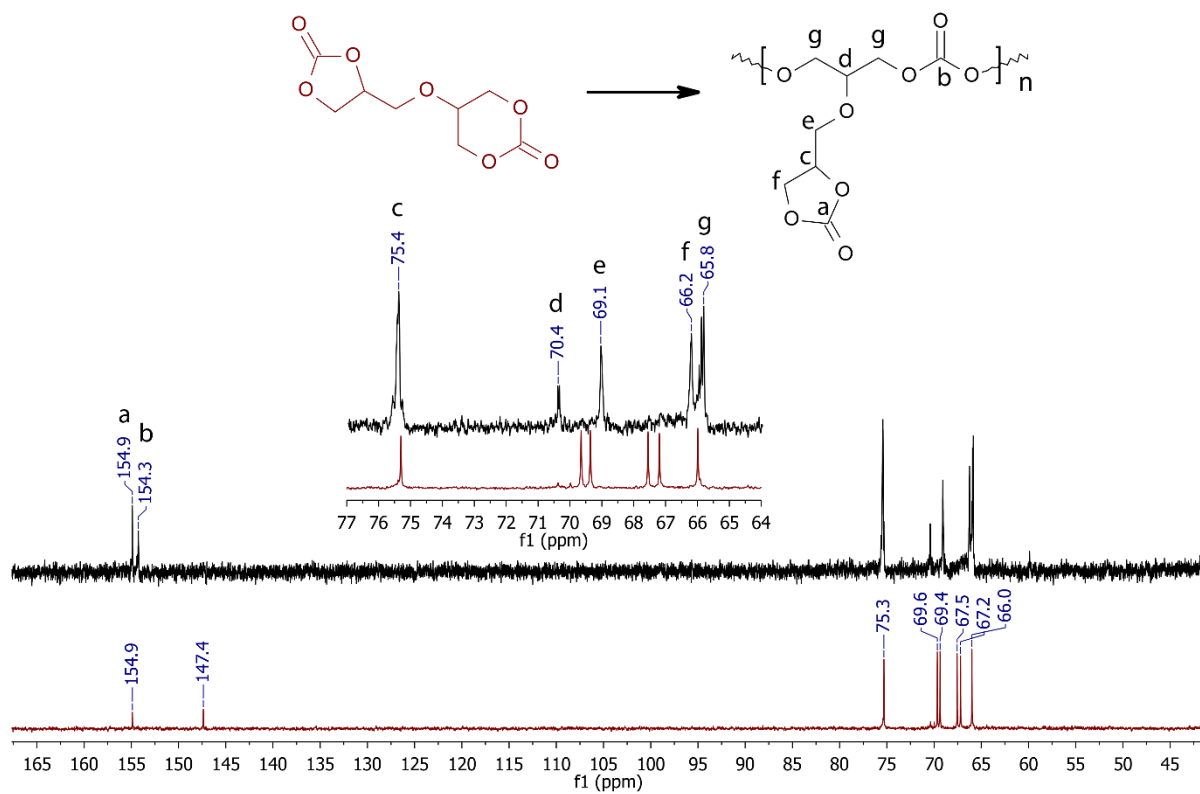


Figure 5S ^{13}C NMR of polycarbonate

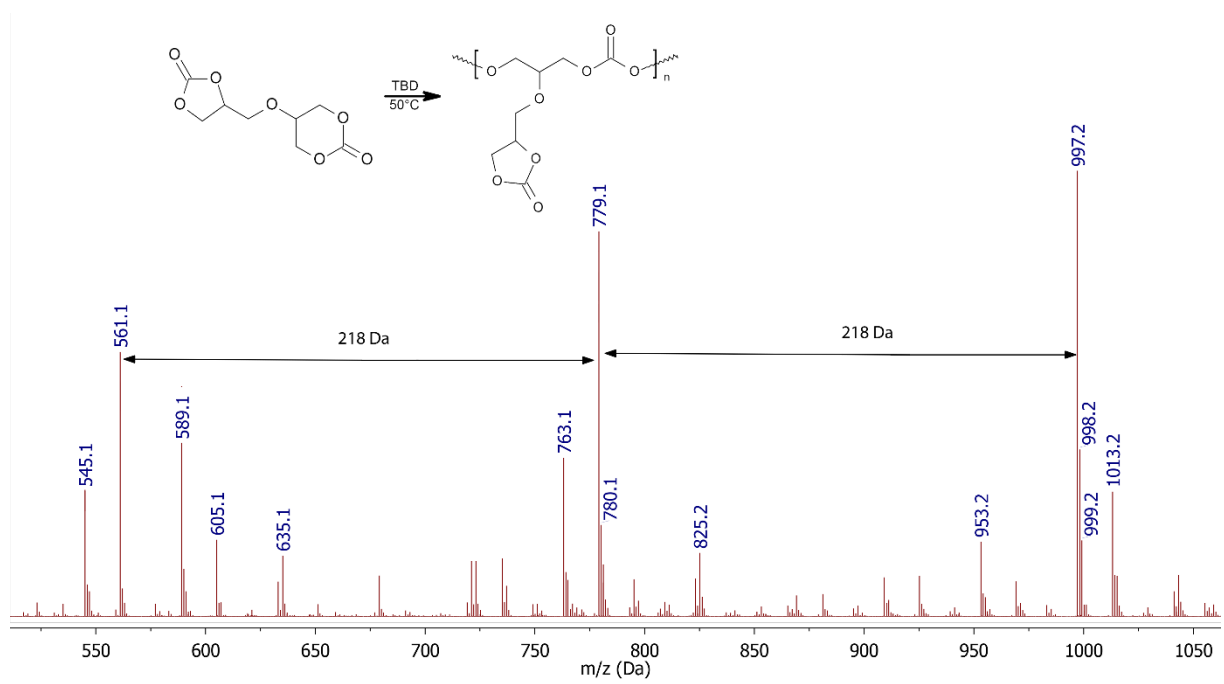


Figure 6S Maldi-ToF of polycarbonate

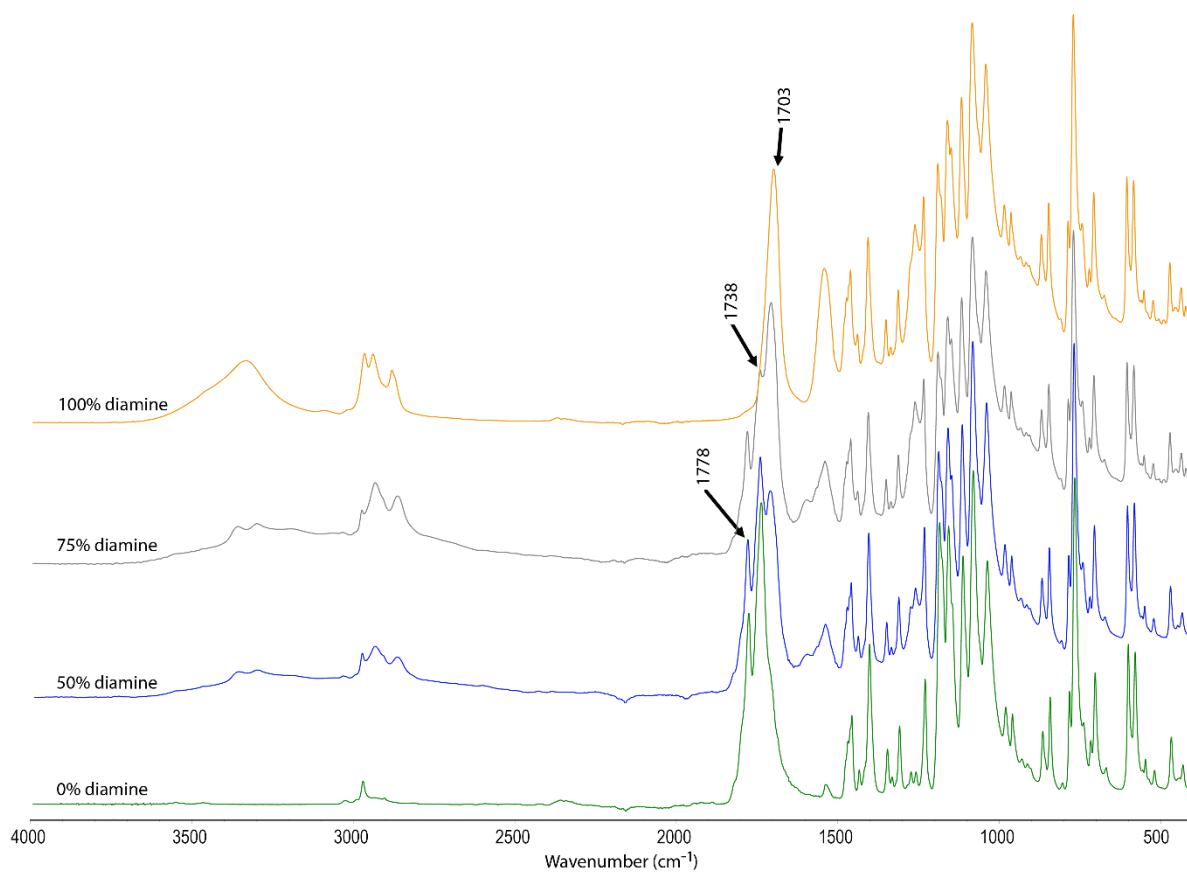


Figure 7S FT-IR of poly(hydroxyurethane)s formation