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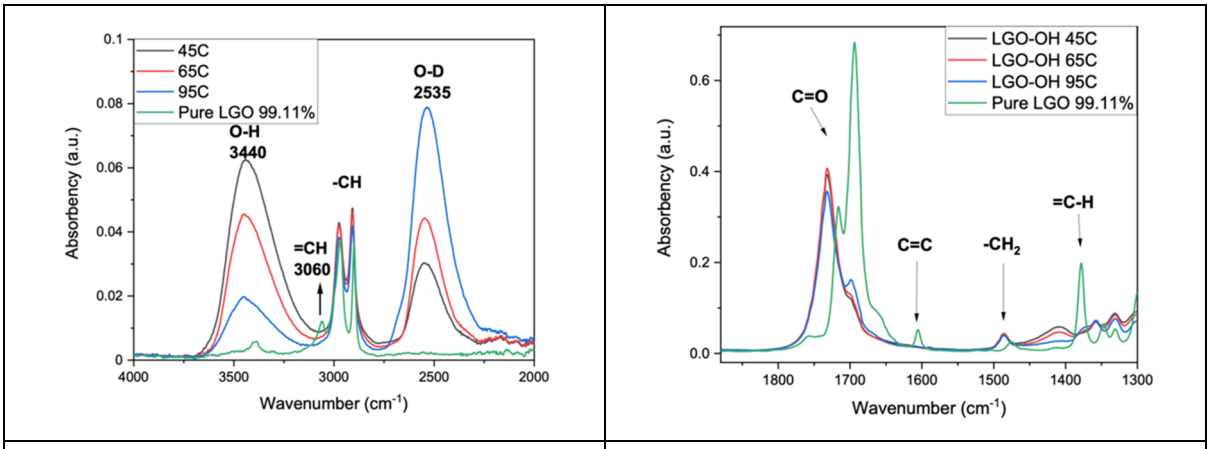
Electronic Supplementary Information (ESI)



A B

Figure S1. IR spectra of LGO and MHC.

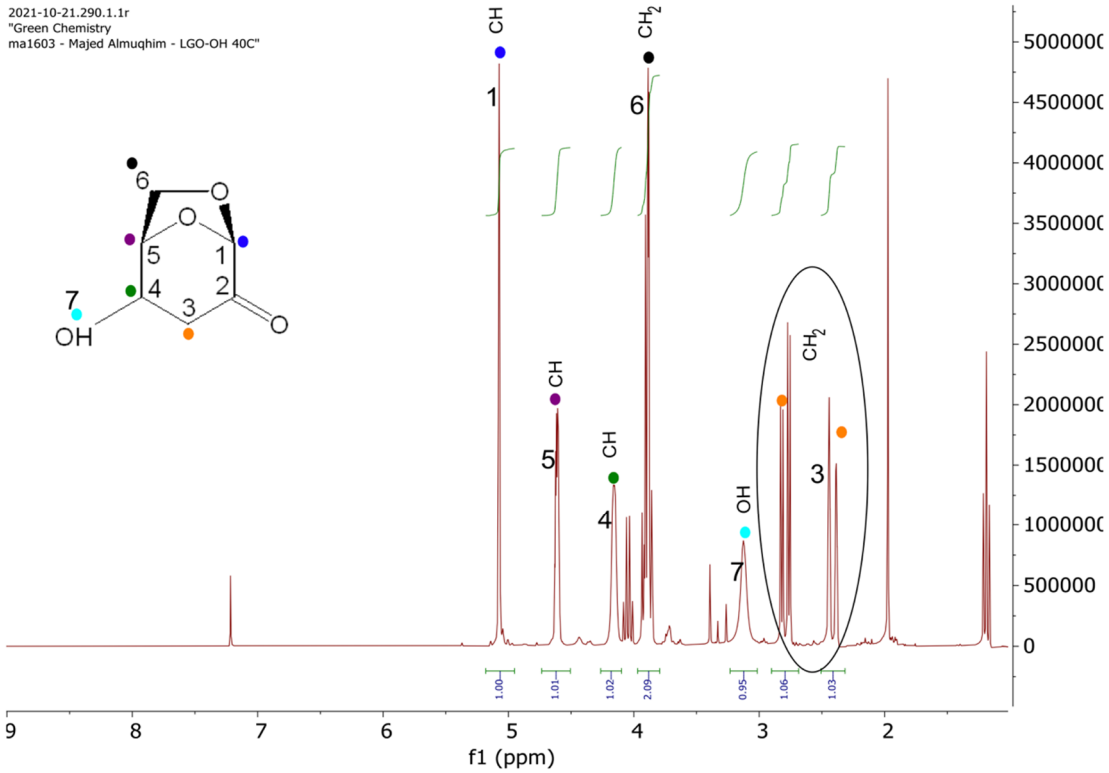
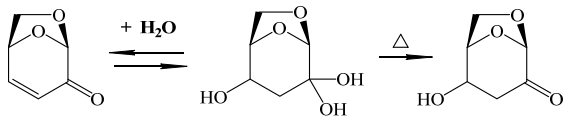
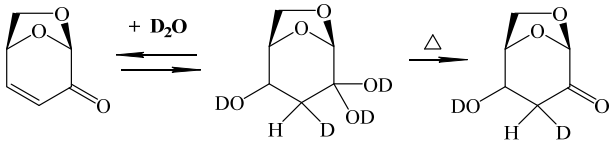


Figure S2. ^{1}H NMR spectrum of MHC.



Molecular Mass 144



Molecular Mass 146

Scheme S1. LGO interaction with H_2O and D_2O.

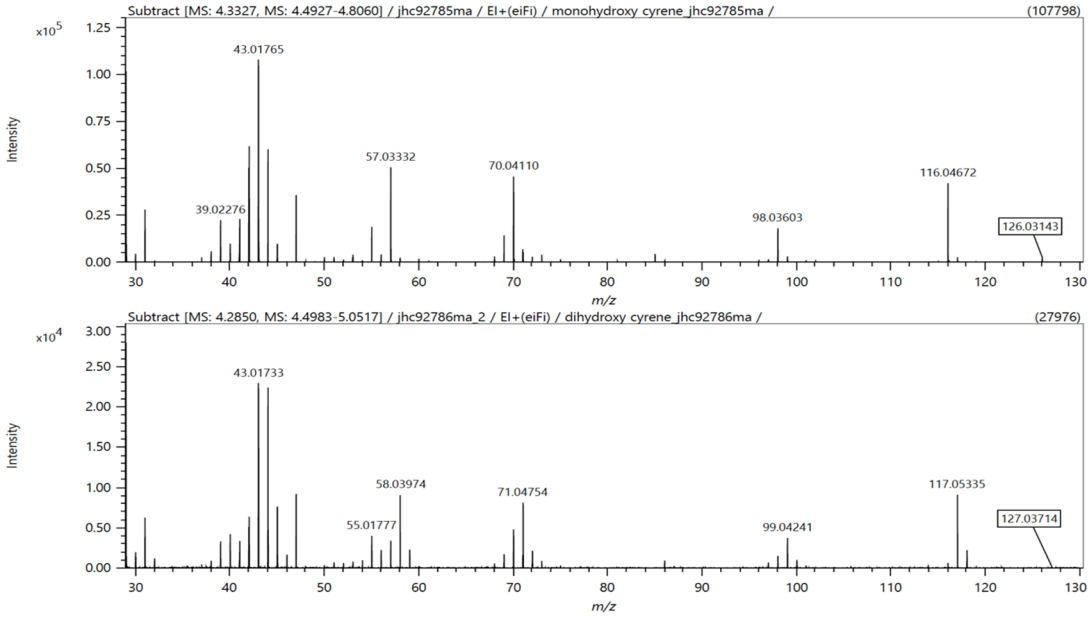


Figure S3. MS of MHC prepared from H_2O (top) and D_2O (bottom).

Table S1. The fragments of the MHC.

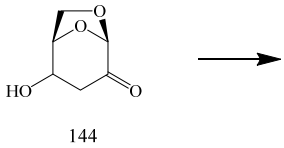
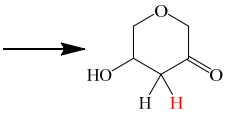
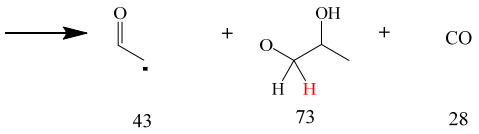
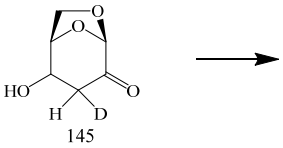
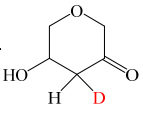
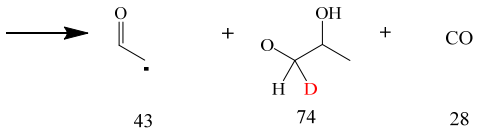
MHC prepared from H_2O	MHC prepared from D_2O
 144  116 + CO 28  43 + 73 + CO 28	 145  117 + CO 28  43 + 74 + CO 28

Table S2. CHN analysis.

	Calculated (%) for				
sample	*C*	*H*	*others*	**MW**	**Formula**
Cyrene					
(test 1)	55.8	6.23	37.97		
(test 2)	55.56	6.11	38.33		
(calculated)	56.25	6.25	37.5	128	$C_6H_8O_3$
LGO					
(test 1)	56.21	5.12	38.67		
(test 2)	56.01	4.99	39.00		
(calculated)	57.14	4.76	38.09	126	$C_6H_6O_3$
LGO-OH 45					
(test 1)	49.12	5.22	45.57		
(test 2)	48.62	5.62	45.76		
(calculated)	50.00	5.56	44.44	144	$C_6H_8O_4$

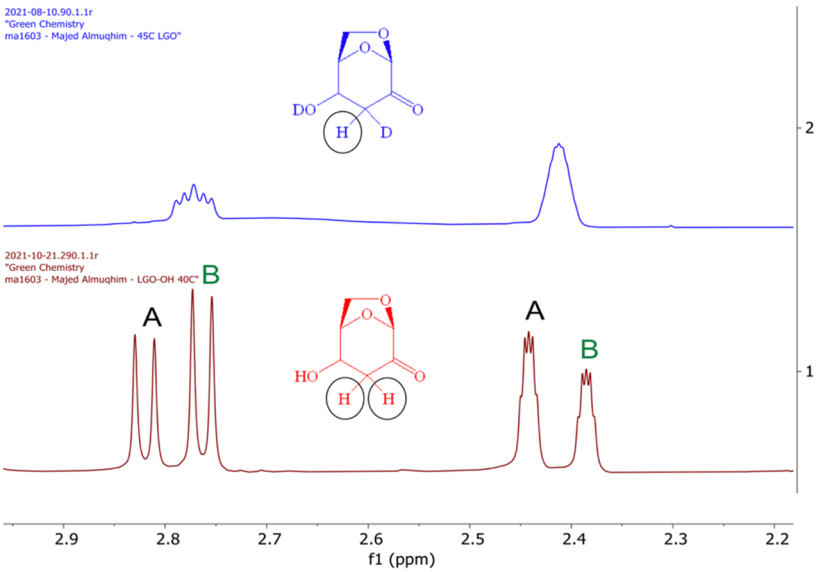


Figure S4. The difference between ^{1}H NMR spectra of MHC prepared from H_2O and D_2O.

Table S3. ^{13}C NMR spectroscopy assessment for MHC.

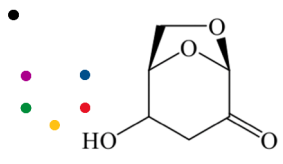
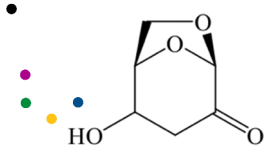
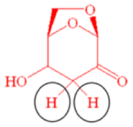
Shift (ppm)	Targeted C	Molecule
101	– **C**< 2O	
70	> **C** – OH	
77.5	– **C**< C,O	
65	O – **C**H$_2$ – C	
40	C – **C**H$_2$ – C	
198	> **C**=O	

Table S4. ^{1}H NMR spectroscopy assessment for MHC.

Shift (ppm)	Targeted proton	Molecule
5.1	– C**H**< 2O	
4.2	> C**H** – OH	
4.7	– C**H**< C,O	
3.8	O – C**H**$_2$ – C	
2.8 2.4	C – C**H**$_2$ – C	

The H_2O attacked the alkene, leaving C3 bonded to two protons

Table S5. integration results for protons on C3 of the MHC prepared from H_2O.

	Isomer A				Isomer B			
Protons on C3 of MHC	ppm	∫	ppm	∫	ppm	∫	ppm	∫
H	2.82	0.45	2.44	0.59	2.76	0.57	2.38	0.41
H in each isomer	1.04				0.98			
Total H	2.02 							

The D_2O attacked the alkene leaving C3 bonded to D in addition to the proton

Table S6. integration results for protons on C3 of the MHC prepared from D_2O.

	Isomer A				Isomer B			
Protons on C3 of MHC	ppm	∫	ppm	∫	ppm	∫	ppm	∫
H	2.77	0.56	--	--	2.41	0.65	--	--
H in each isomer	0.39				0.58			
Total H	0.97 							

Calculating the protons positions for the C3

NMR field = 300 M Hz
∴ 1 ppm = 300 Hz

J value =
2.83 – 2.77 = 0.06 ppm x 300 = 18 Hz
2.83 – 2.81 = 0.02 ppm x 300 = 6 Hz
2.39 – 2.386 = 0.0034 ppm x 300 ≈ 1 Hz
2.39 – 2.38 = 0.001 ppm x 300 = 3 Hz (total multiplet)

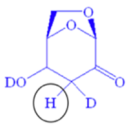
Additionally, one of the two protons on C3 (at ~ 2.4 ppm) is coupled with the proton on C5 as seen by ^{1}H COSY NMR spectroscopy using the W conformation.[18] This is highlighted by the red bonds illustrated in figure (5 D).

The MHC results show that they match the MHC theoretical calculations. Cyrene and LGO were tested, and their results also matched the theoretical calculations.

Table S7. integration results for protons on C3 of the MHC prepared from H_2O.

Protons on C3 of MHC	ppm	∫	ppm	∫	ppm	∫	ppm	∫
H	2.82	0.45	2.44	0.59	2.76	0.57	2.38	0.41
H in each position	1.04				0.98			
Total H	2.02							

Table S8. integration results for protons on C3 of the MHC prepared from D_2O.

Protons on C3 of MHC	ppm	∫	ppm	∫	ppm	∫	ppm	∫
H	2.77	0.56	--	--	2.41	0.65	--	--
H in each position	0.39				0.58			
Total H	0.97							

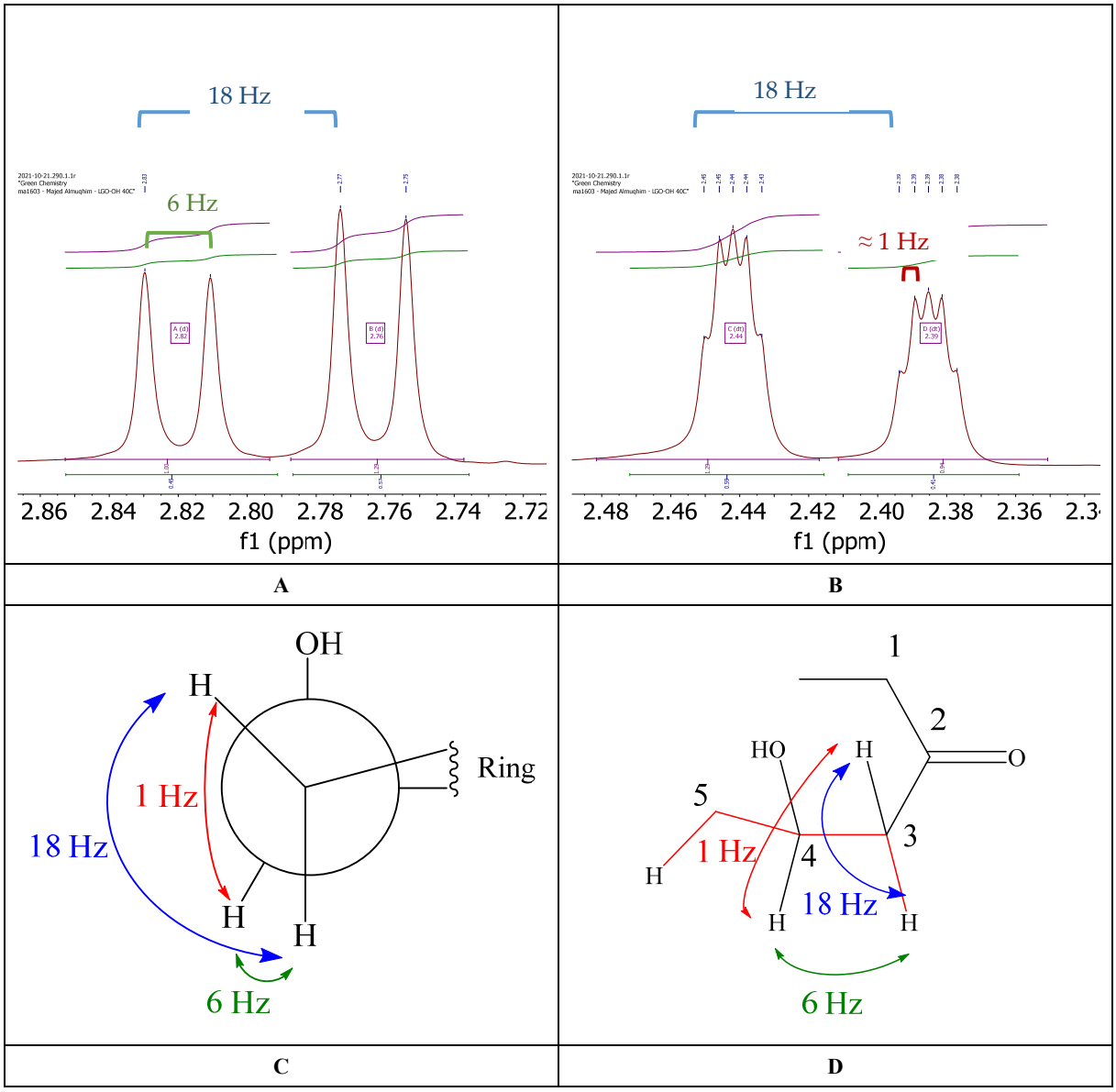


Figure S5. Protons coupling on C3.

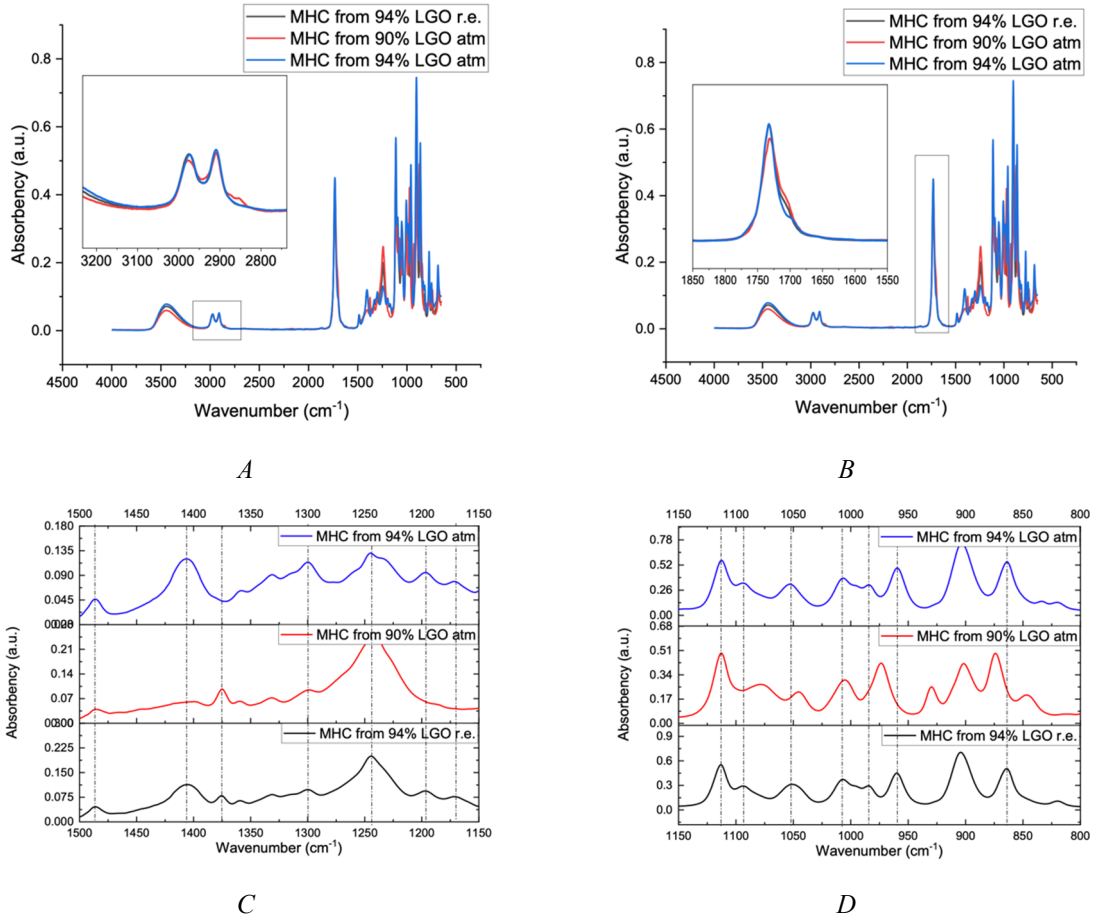


Figure S6. Spectra of MHC in different water sources and production methods.

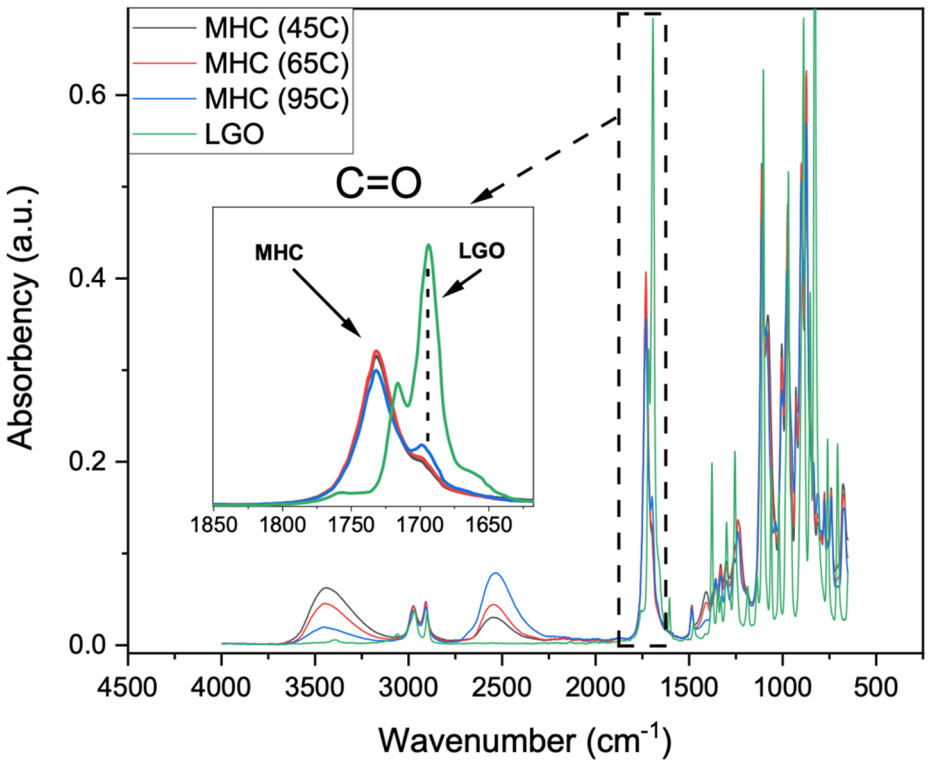


Figure S7. IR spectra for MHC prepared in different temperatures.

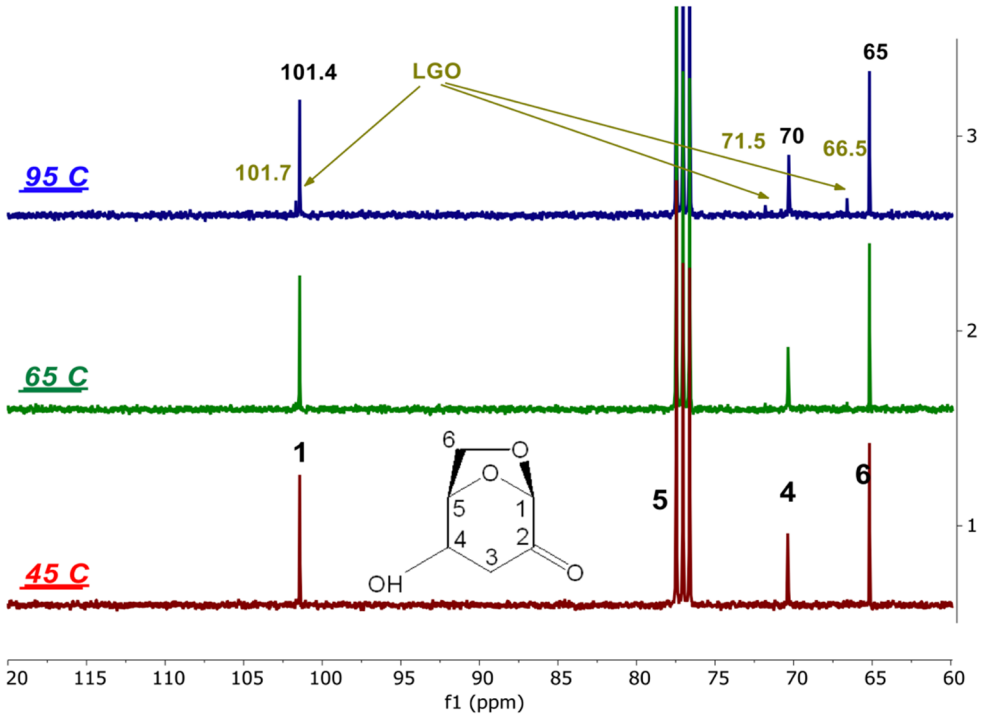


Figure S8. ^{13}C NMR spectra for MHC prepared in different temperatures.

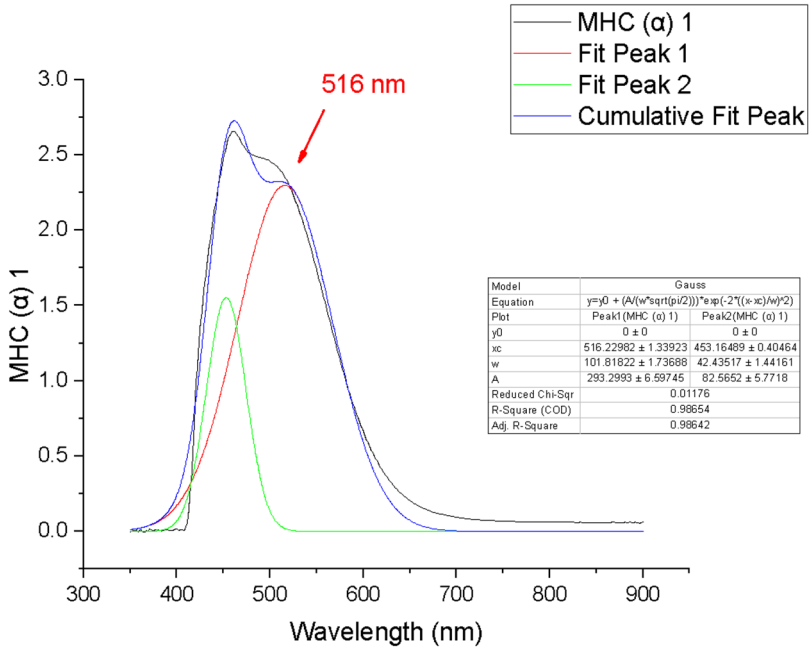


Figure S9. UV-Vis spectra of Reichardt's dye in the presence of MHC (deconvoluted bands).

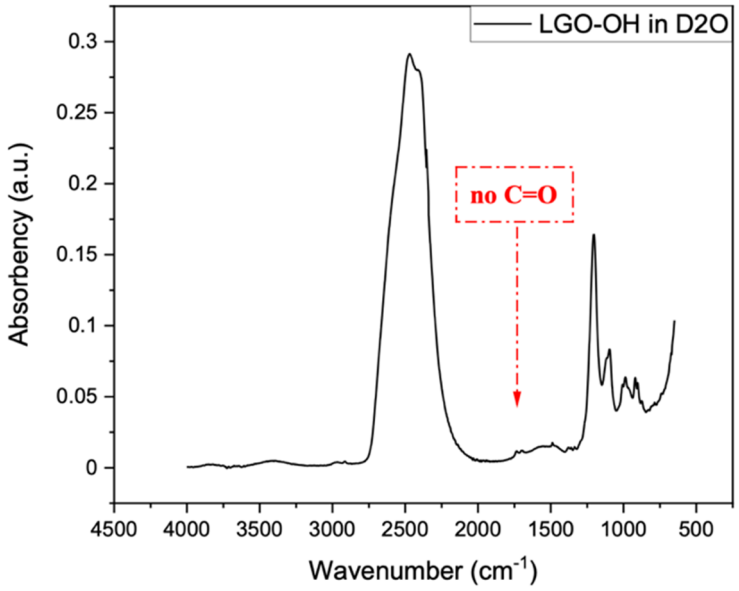
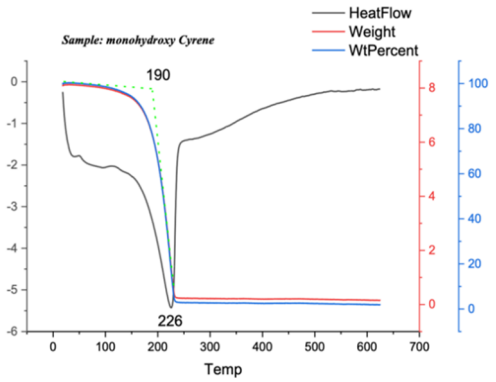
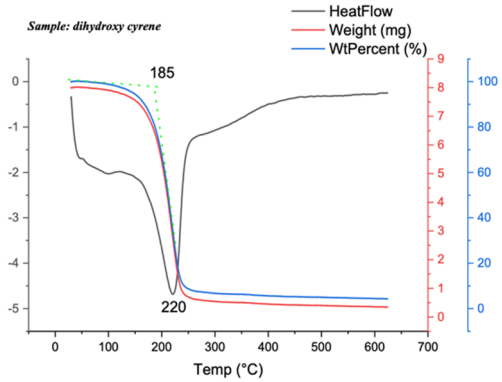


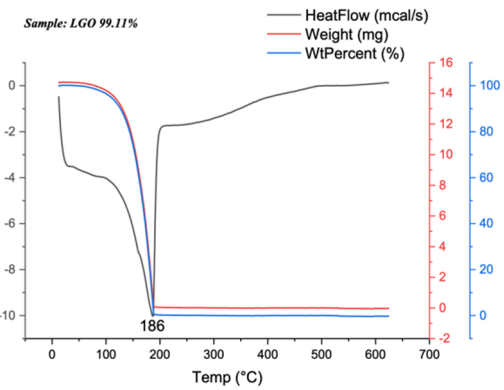
Figure S10. IR spectrum of 10% MHC in D_2O shows no vibration band for the ketone.



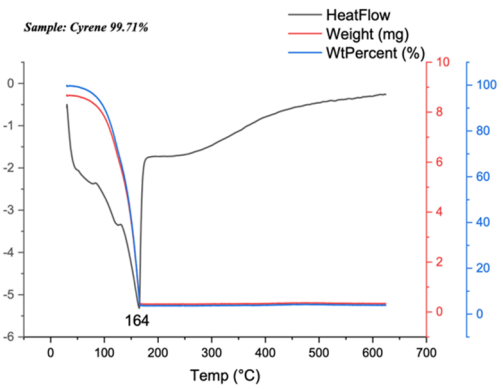
MHC From H_2O EtOAc extraction



MHC From D_2O MHC 65C

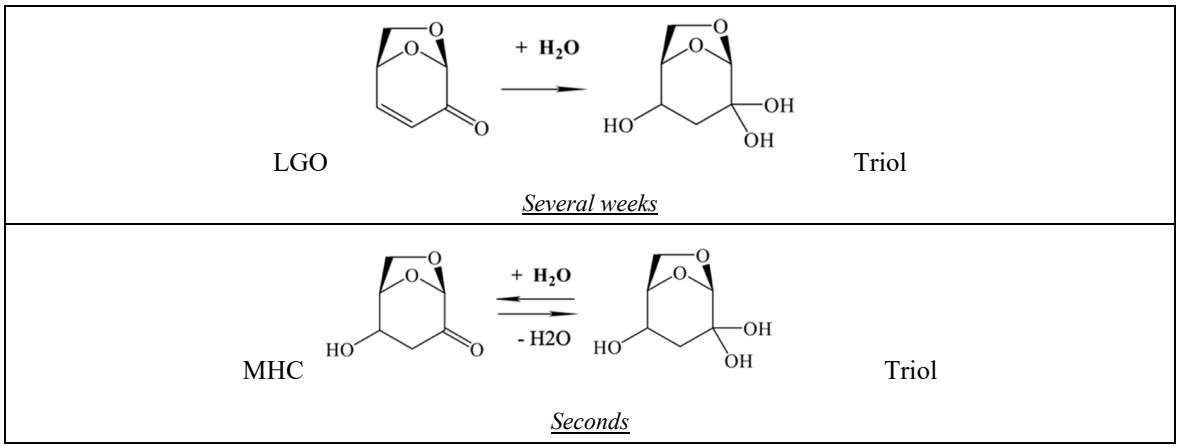


LGO



Cyrene

Figure S11. MHC has higher boiling point than both Cyrene and LGO.



Scheme S2. The difference between LGO and MHC in water.

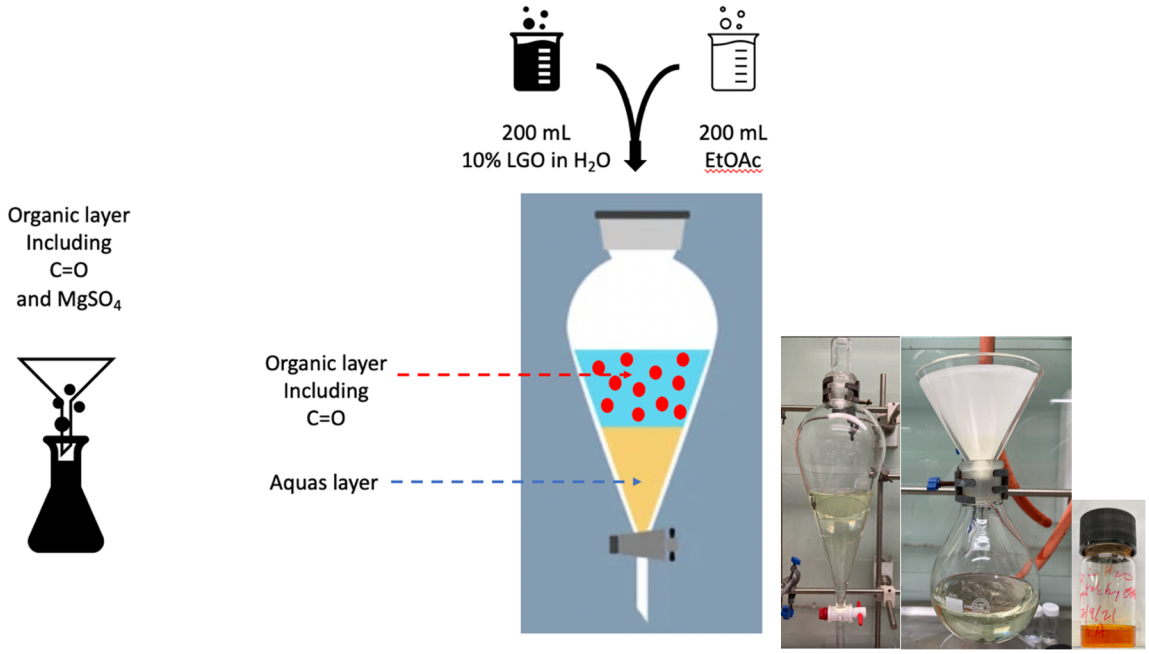


Figure S12. EtOAc extraction method.

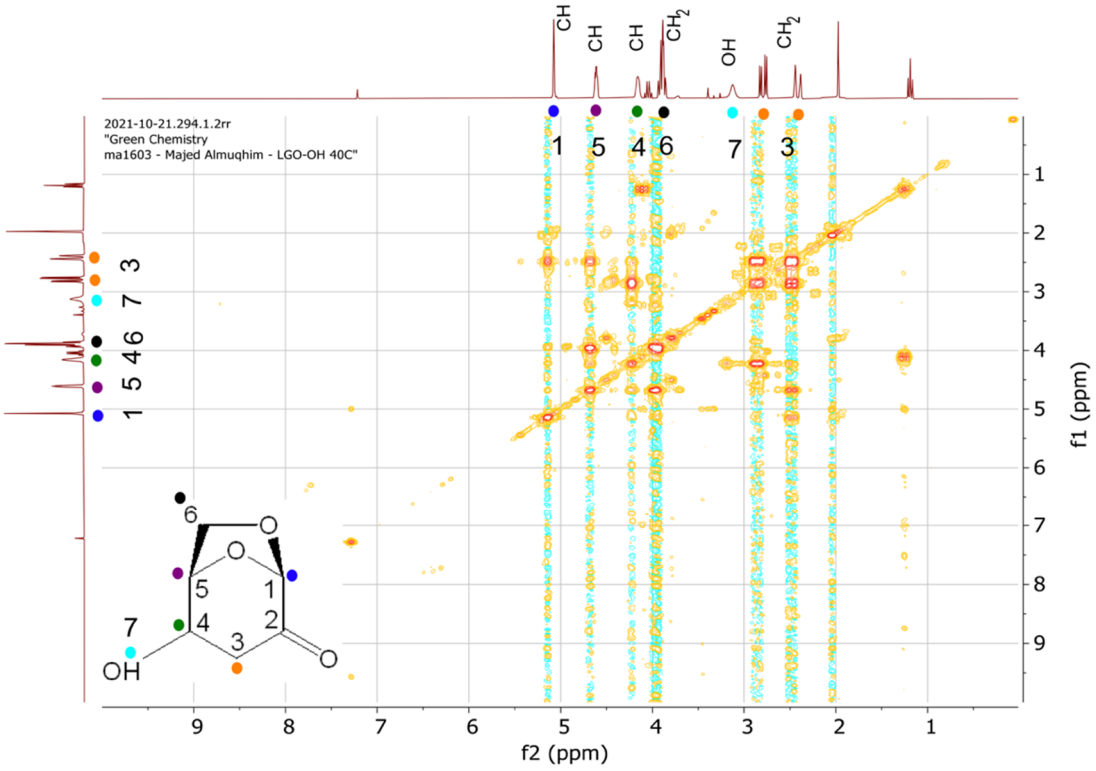


Figure S13. ^{1}H COSY NMR spectrum for MHC in $CDCl_3$. The MHC was produced from LGO dissolved in H_2O.

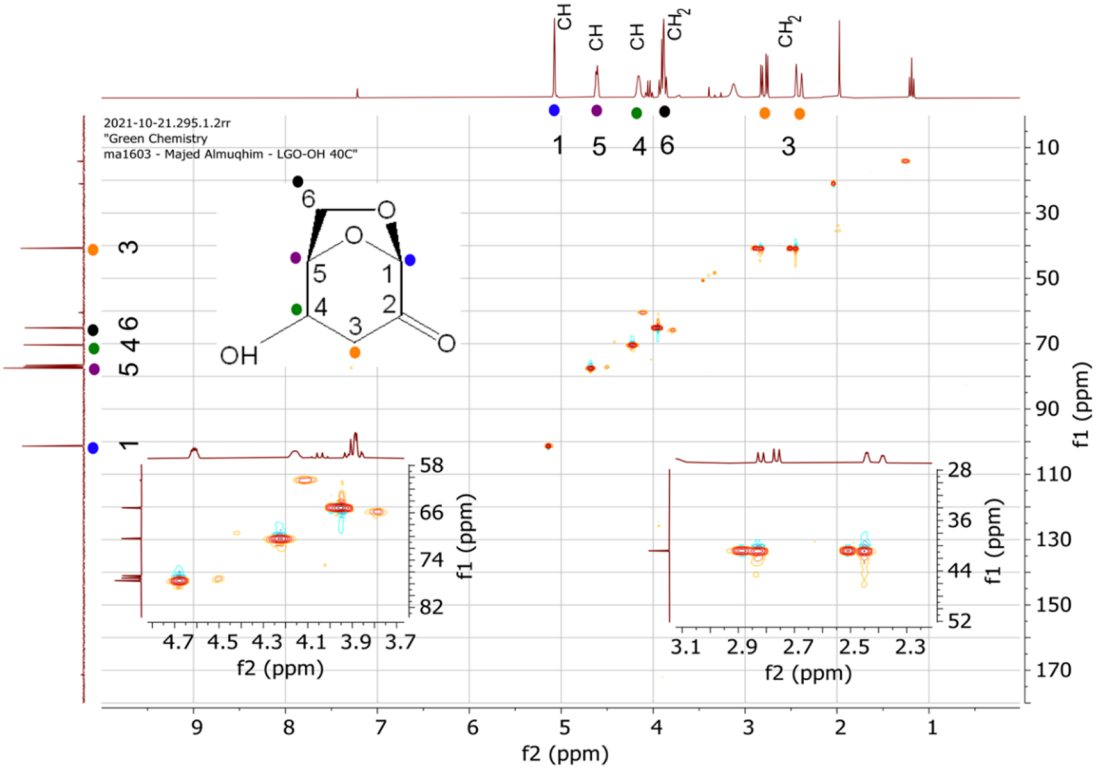


Figure S14. 2D ^{1}H+^{13}C HSQC NMR spectrum for MHC in $CDCl_3$. The MHC was produced from LGO dissolved in H_2O.

As shown in Figure (S15) there is no significant change during cooling process. The minimum temperature for the instrument was – 60 °C. Therefore, the melting point is below – 60 °C.

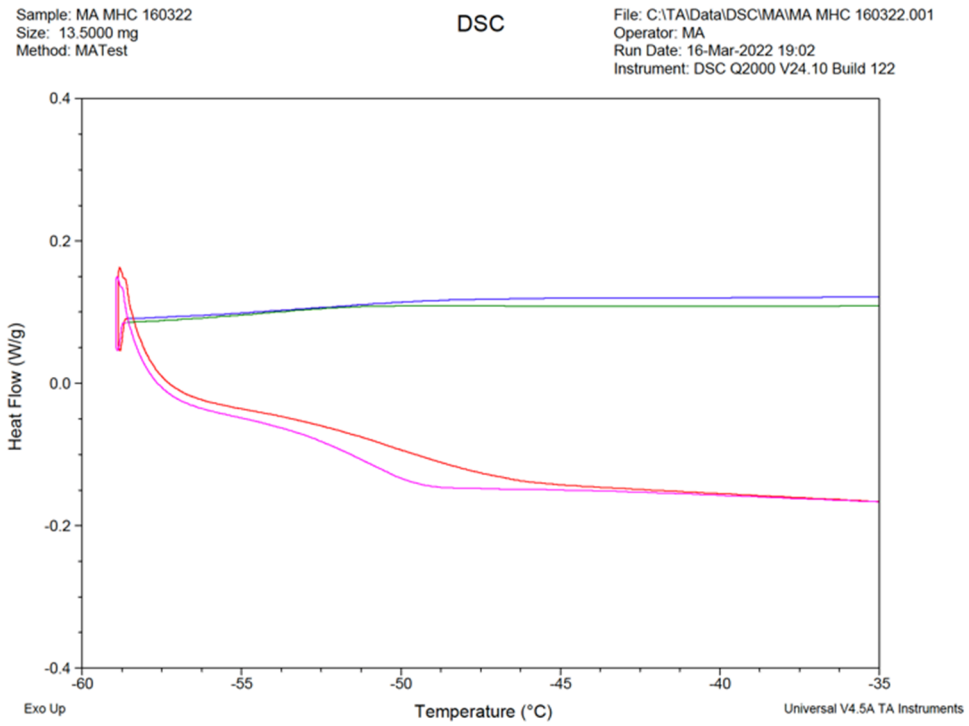


Figure S15. DSC for MHC.

3D modelling for MHC using COSMO

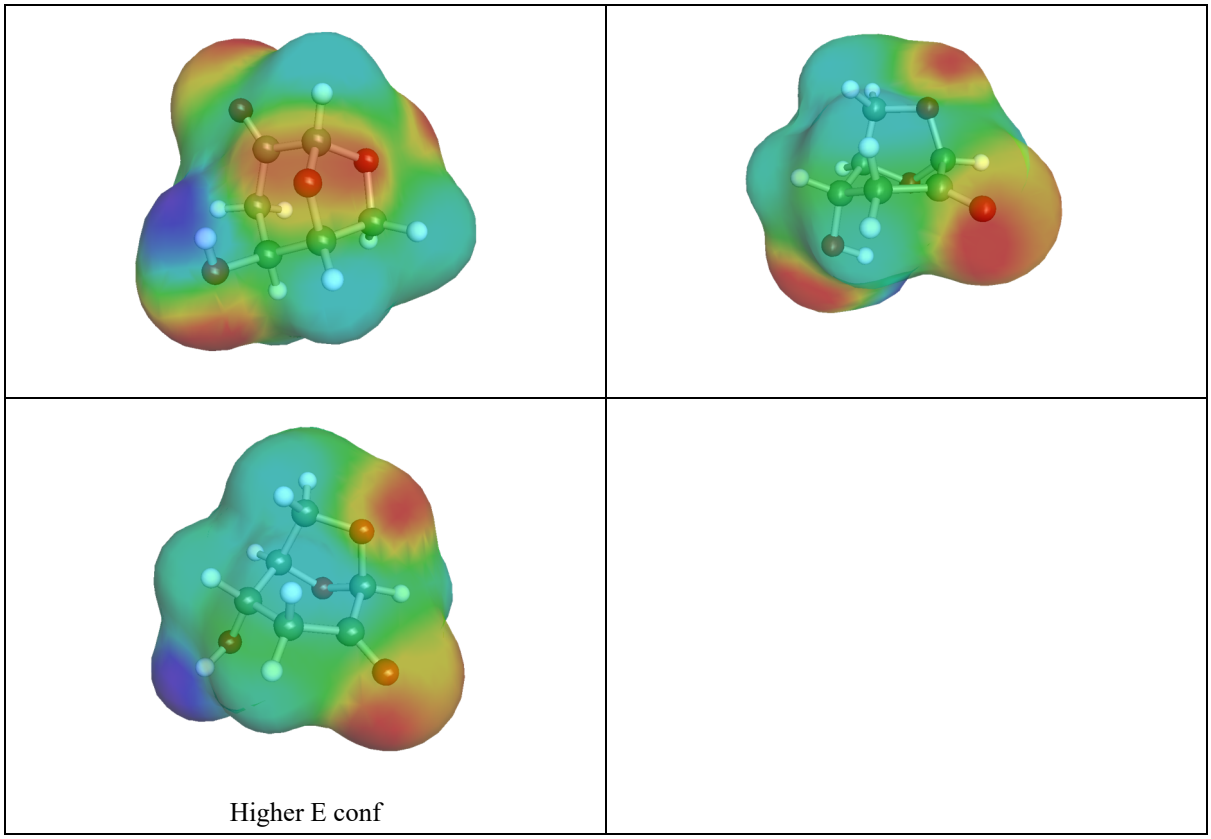


Figure S16. shows 3D modelling using COSMO to identify the intramolecular H-bonding for MHC, in different electronic configurations.