Supplementary Information

Kinetic Evaluation of Chitosan Derived Catalysts for the Aldol Reaction in Water

Anton De Vylder[a], Jeroen Lauwaert[b], Jeriffa De Clercq[b], Pascal Van Der Voort[c], Christian V. Stevens[d], Joris W. Thybaut[a,*]

[a]Laboratory for Chemical Technology (LCT), Department of Materials, Textiles, and Chemical Engineering, Ghent University, Technologiepark 125, 9052 Ghent, Belgium

[b]Industrial Catalysis and Adsorption Technology (INCAT), Department of Materials, Textiles, and Chemical Engineering, Ghent University, Valentin Vaerwyckweg 1, 9000 Ghent, Belgium

[c]Center for Ordered Materials, Organometallics and Catalysis (COMOC), Department of Chemistry, Ghent University, Krijgslaan 281-S3, 9000 Ghent, Belgium

[d]SynBioC Research Group, Department of Green Chemistry and Technology, Ghent University, Coupure Links 653, 9000 Ghent, Belgium

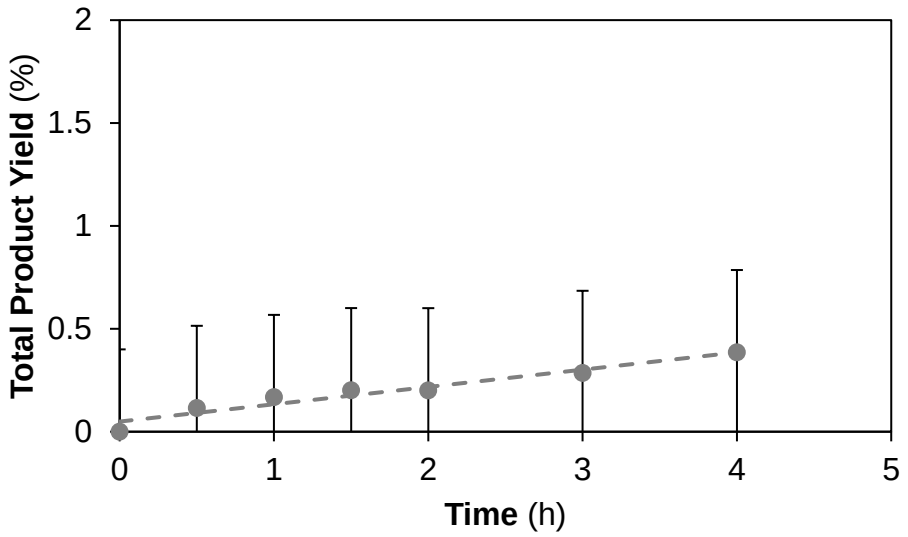

Figure 1S: measured total product yield versus reaction time when no catalyst is used. (T = 55 °C, $m_{acetone}$ = 45 g, m_{4NB} = 0.45 g, m_{water} = 55 g)

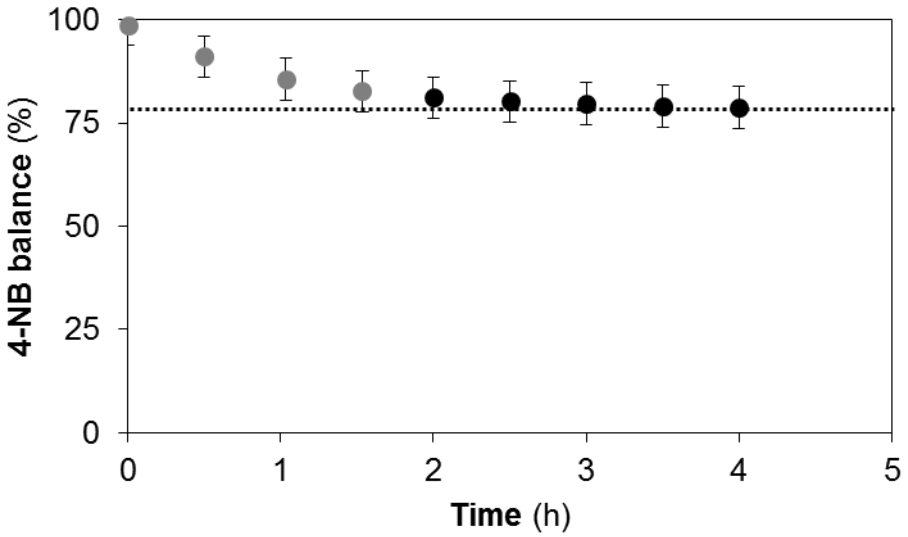

Figure 2S: 4-nitrobenzaldehyde molar balance versus reaction time for crude low-molecular weight chitosan as catalyst in the aldol reaction of acetone with 4-nitrobenzaldehyde. (T = 55 °C, $m_{acetone}$ = 45 g, m_{4NB} = 0.45 g, m_{water} = 55 g, m_{cat} = 0.26 g)

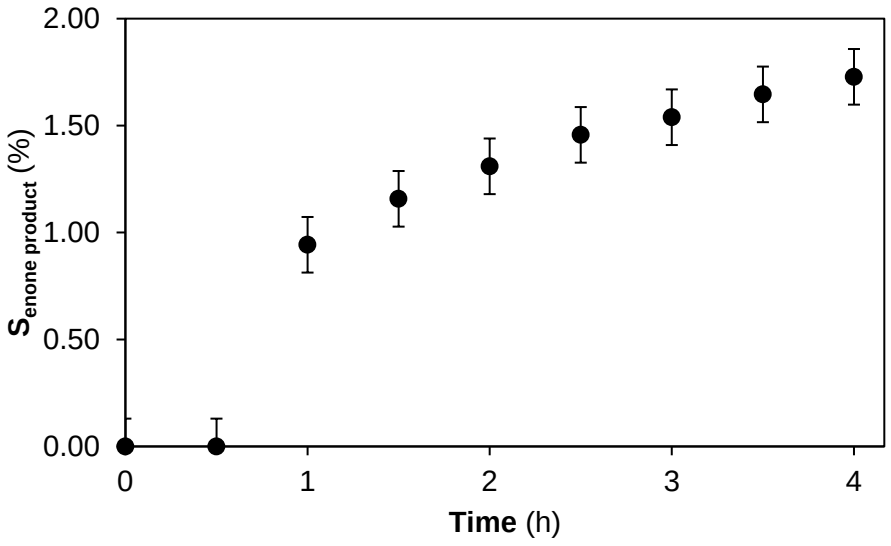

Figure 3S: Enone product selectivity as a function of time for the chitosan hydrogels. The product selectivity graphs for the other catalyst morphologies are similar. The aldol product selectivity is the inverse of the enone product selectivity.

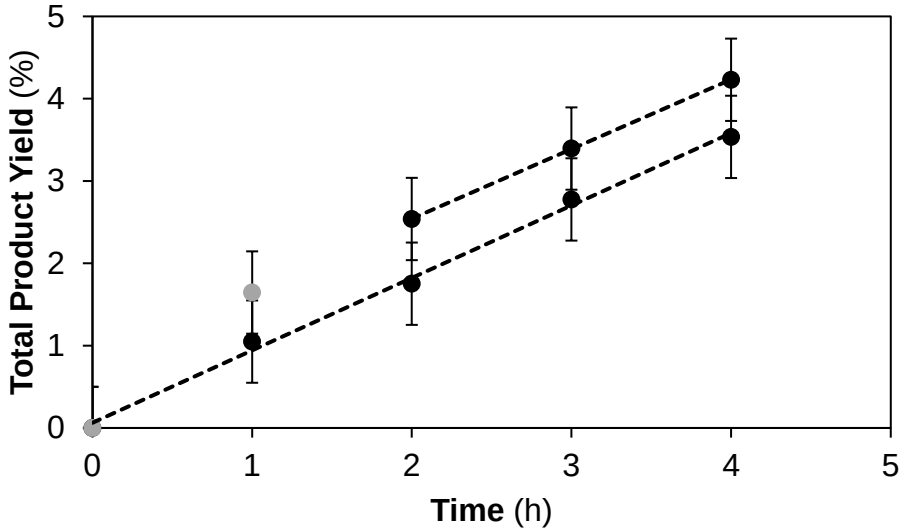

Figure 4S: measured total product yield versus reaction time for low-molecular weight chitosan hydrogel as catalyst in the aldol reaction of acetone with 4-nitrobenzaldehyde in a small scale reaction. (T = 55 °C, $m_{acetone}$ = 22.5 g, m_{4NB} = 0.225 g, m_{water} = 27.5 g, $m_{chitosan}$ = 0.05 g)

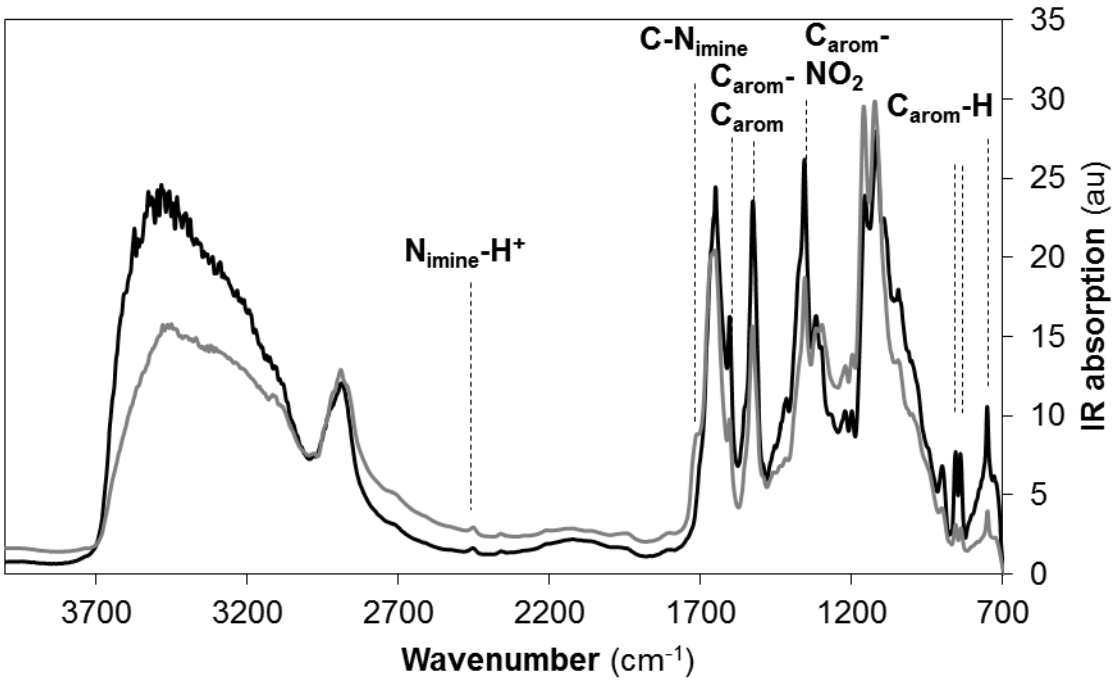

Figure 5S: DRIFTS spectrum of chitosan reacted with 4-nitrobenzaldehyde in a 45g DMSO, 55g water mixture at 55 °C (black) compared to the catalyst spent in the aldol reaction (grey).