

Depolymerization of cellulosic feedstocks using magnetically separable functionalized graphene oxide

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Supporting Information

Estimation of activation energy

Activation energy of the reaction was calculated using Arrhenius equation. Half-life time ($t_{1/2}$) at different temperatures was recorded for calculate activation energy.

$$k = Ae^{-E_a/RT} \quad \text{--- Eq. 1}$$

Where k is the reaction rate coefficient, A is the frequency factor for the reaction, R is the universal gas constant (8.314J/K/mol) and T is the temperature (in kelvin).

T (K)	1/T	k(h ⁻¹)	lnk
348	0.002874	0.060	-2.81341
373	0.002681	0.079	-2.53831

The activation energy was found algebraically by substituting two rate constants (k_1 , k_2) and the two corresponding reaction temperatures (T_1 , T_2) into the two-point form of the Arrhenius Equation (2).

$$E_a = \frac{R T_1 T_2}{(T_1 - T_2)} \ln \frac{k_1}{k_2} \quad \text{--- Eq. 2}$$

Figure S1: A representative chromatogram of HPLC analysis for hydrolyzed microcrystalline cellulose.

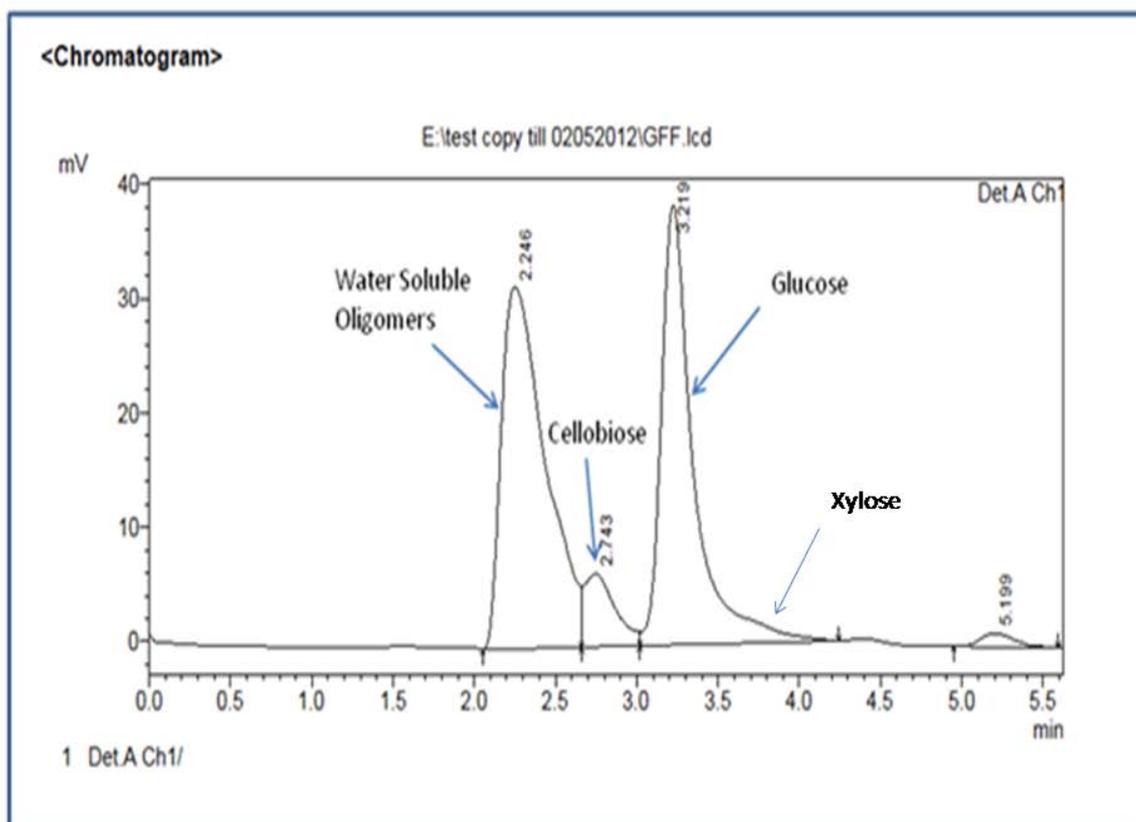


Figure S2: NMR of water soluble hydrolysis products for Fe-GO catalyst.

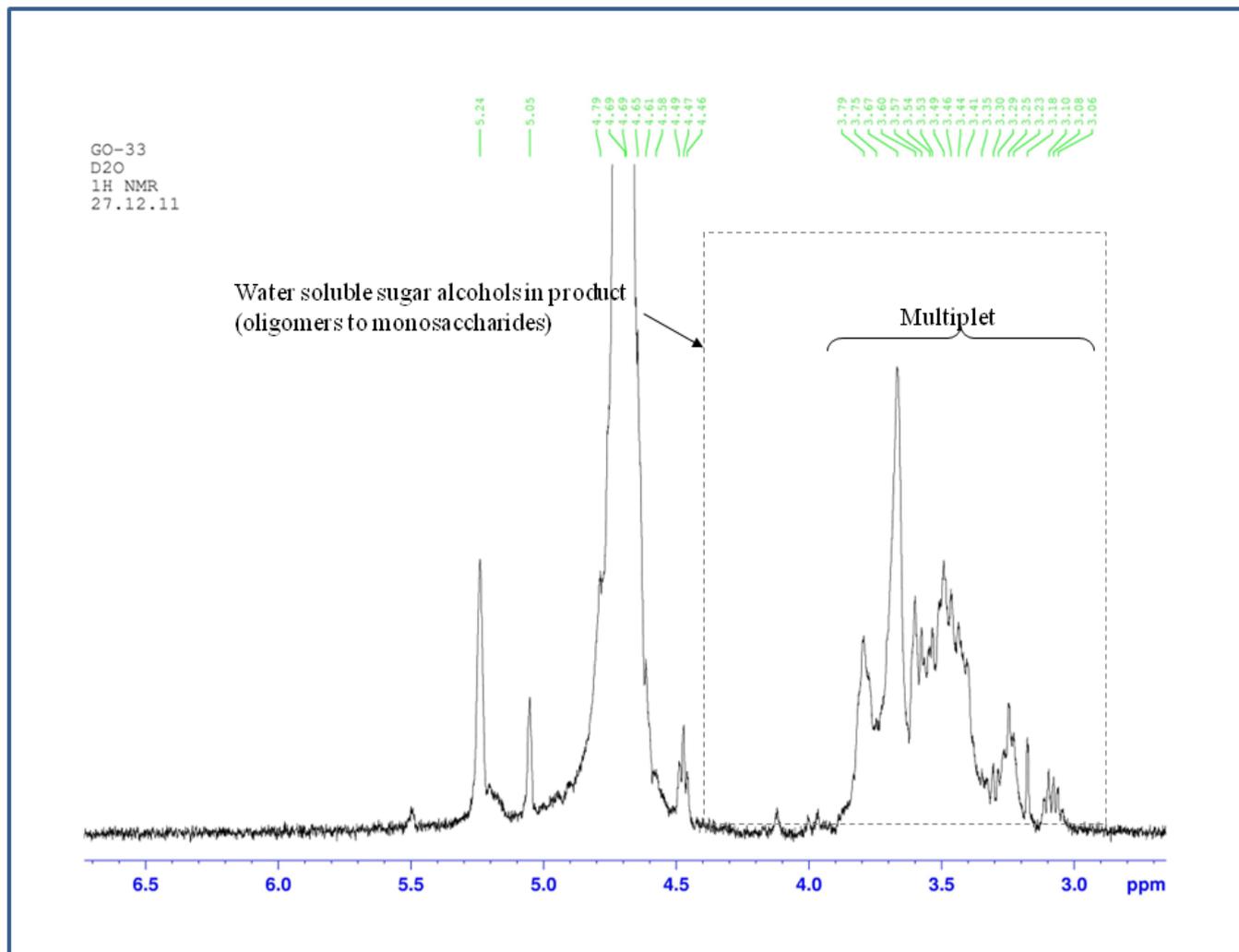


Figure S3: MALDI-TOF-MS for the reaction solution. $m/z = 162$ represents the mass number of glucose monomer $[-(-O-C_6H_{10}O_4)-]_n$ in β -1,4 glucan.

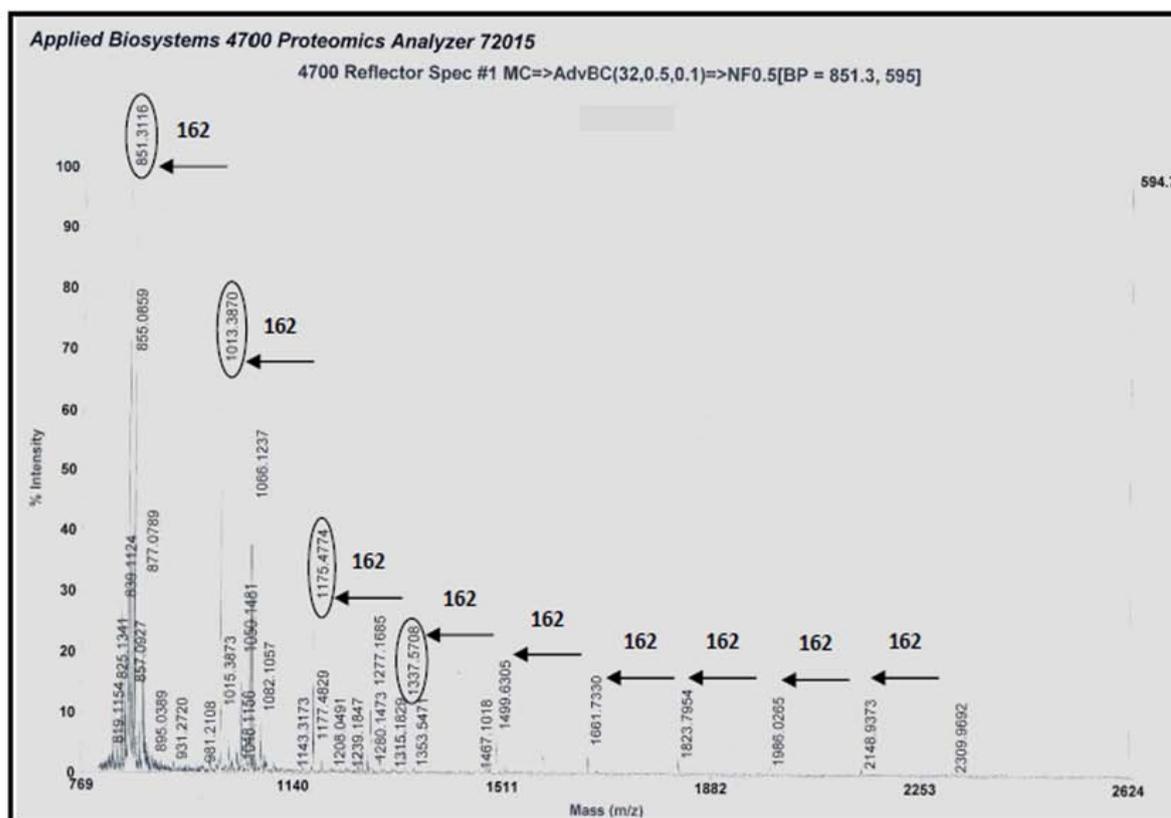
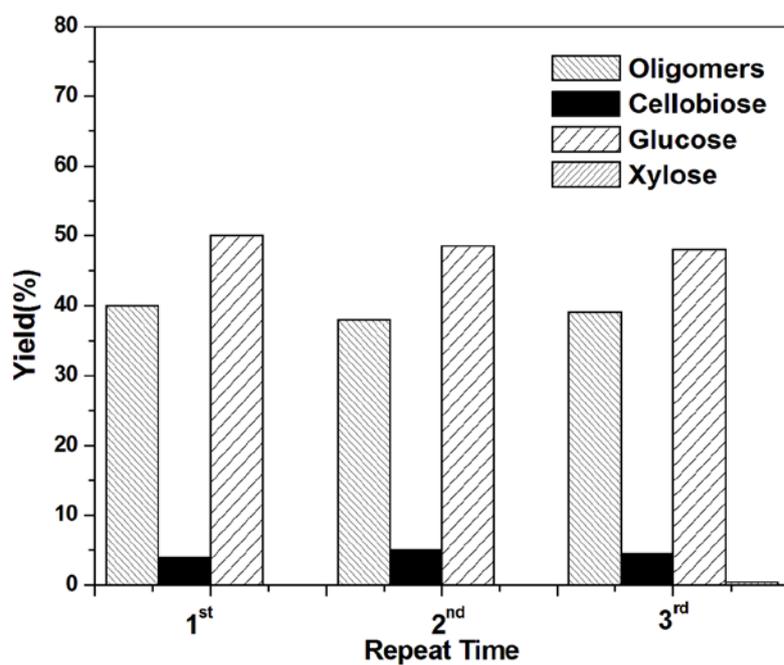
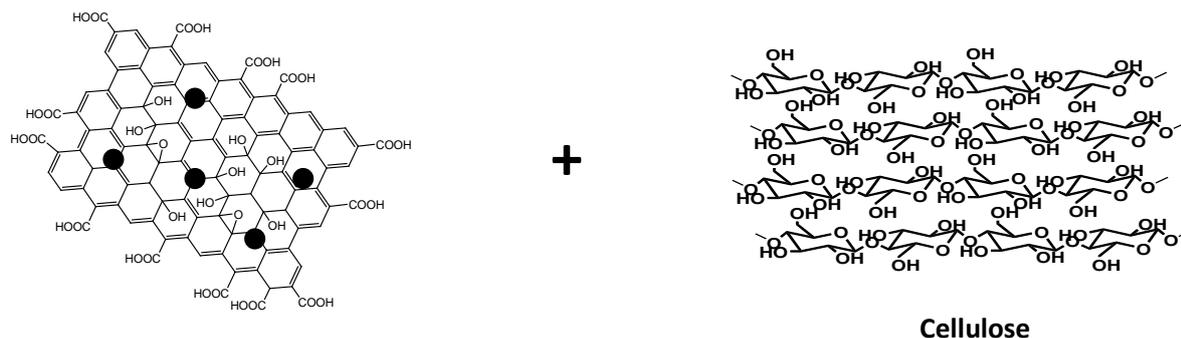


Figure S4: Recycling activity for the hydrolysis of crystalline cellulose with functionalized magnetic graphene oxide Fe-G-SO₃H (reaction time=44h).



Supporting Scheme 1: Mechanistic steps involved in the hydrolysis of cellulose into water soluble carbohydrates.



Fe-Graphene Oxide (Fe-GO)

[1.6mmol/g_{cat.} (-COOH),
0.6mmol/g_{cat.} (-OH)]

Catalysts having polar groups (-COOH, -OH) on its surface and these groups adhere on the surface of microcrystalline cellulose which is also having polar group (-OH) through H-bonding.

-COOH groups create a gap between polymeric cellulose layers, by attack on β -1,4 glycosidic linkage of cellulose to form oligosaccharides, followed by hydrolysis of β -1,4 glycosidic bonds in oligosaccharides.

