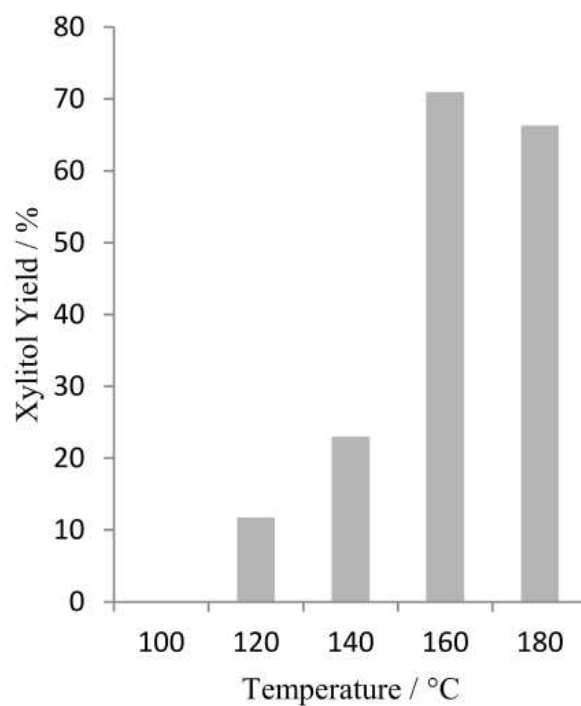


# One-pot Selective Conversion of Hemicellulose to Xylitol

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## 1. Effect of Temperature



**Figure S1:** Yield of xylitol with Ru/C at different temperatures for phosphotungstic acid. Reaction conditions: xylan (0.075 g); Ru/C (0.025 g);  $H_3PW_{12}O_{40}$ ; (0.100 g); water (8.0 mL);  $H_2$  (20 bar); 5 min.

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## 2. Calibrations

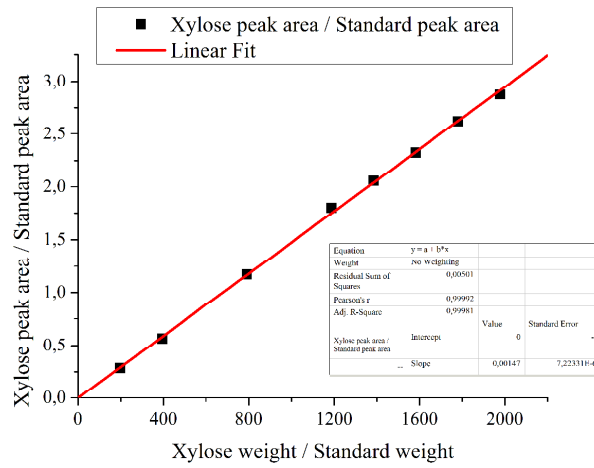
Xylose, xylitol and arabinose yields were determined via HPLC peak areas based on the calibration of pure samples with ethylene glycol as external standard. Due to very close retention times in the HPLC, separation of xylan and sugar oligomers was not possible. The negligible amount of arabitol in xylitol was not separately quantified. Table S1 is an overview of the product concentrations in case of 100 % yield ( $n(\text{product}) = n(\text{xylan})$ ). Equation 1 shows the calculation of yields based on the mass concentration  $c_m$ .

$$\text{Yield (\%)} = \frac{c_m \text{ (g/L)}}{c_m^{\text{max}} \text{ (g/L)}} \cdot 100 \quad (1)$$

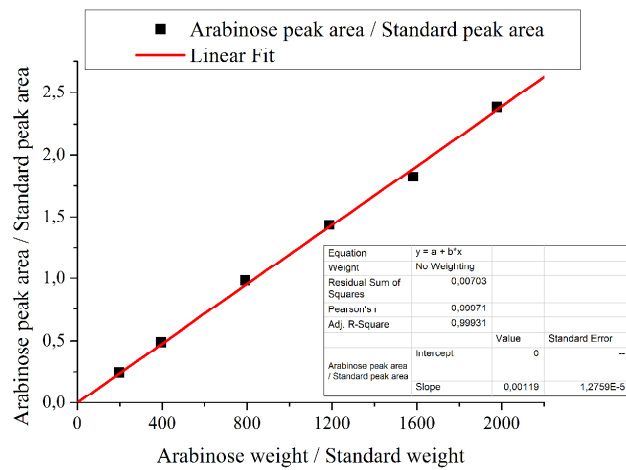
$c_m$  of xylose, arabinose and xylitol were calculated using equation 2.

$$c_m \text{ (g/L)} = \frac{\text{peak area compound}}{\text{peak area standard}} \cdot \text{calibration factor} \quad (2)$$

The calibration factor is the slope of the compound weight per standard weight plotted against the corresponding compound peak area per standard peak area (figures S2-S4) multiplied by the standard weight (5.1 mg).

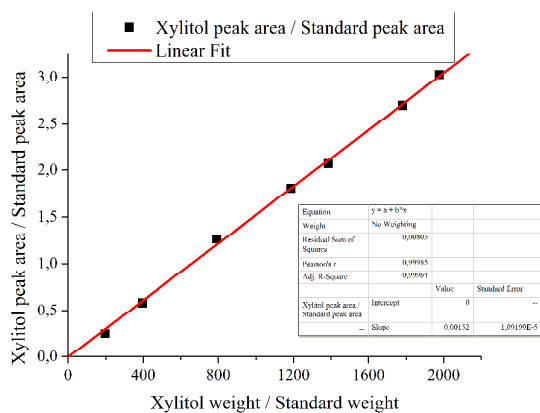


**Figure S2:** Xylose calibration with calibration samples (1; 2; 4; 6; 7; 8; 9; 10 g/L) and 5.1 mg standard.



**Figure S3:** Arabinose calibration with calibration samples (1; 2; 4; 6; 8; 10 g/L) and 5.1 mg standard.





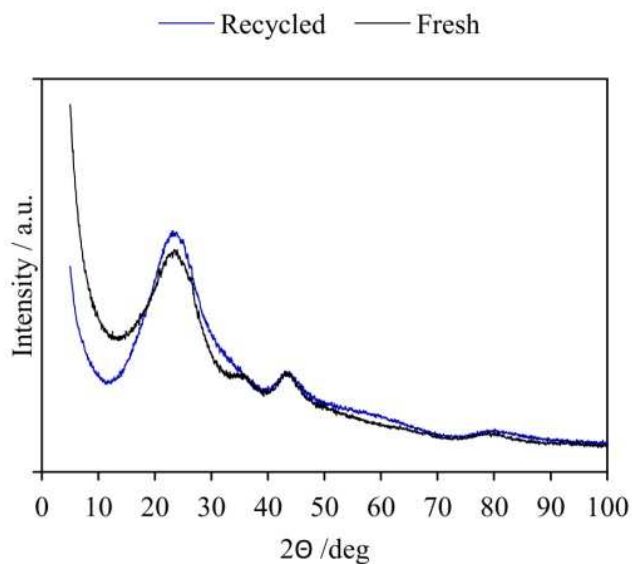
**Figure S4:** Xylitol calibration with calibration samples (1; 2; 4; 6; 7; 9; 10 g/L) and 5.1 mg standard.

**Table S1:** Overview of identified products and maximum product concentrations.

Reaction condition	Compound	M (g/mol)	m <sup>max</sup> (mg)	n <sup>max</sup> (mmol)	V (mL)	cm (g/L)
(1)	Xylan	132.11	100.0			10.0
	Xylose	150.13	113.6			11.4
	Arabinose	150.13	113.6			11.4
	Xylitol	152.15	115.2			11.5
	Arabitol	152.15	115.2	0.757	10.0	11.5
(2)	Xylan		75.00			9.38
	Xylose		85.23			10.7
	Arabinose		85.23	0.568	8.0	10.7
	Xylitol		86.38			10.8
	Arabitol		86.38			10.8
(2a) 0.6 mL LA					8.60	10.0
(2b) 0.4 mL LA					8.40	10.3
(2c) 0.25 mL LA	Xylitol		86.38		8.25	10.5
(2d) 0.1 mL LA					8.10	10.7
(2e) 0.05 mL LA					8.05	10.7

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### 3.1 X-ray Diffraction pattern



**Figure S5:** X-ray diffraction patterns of fresh and recycled Ru/C.

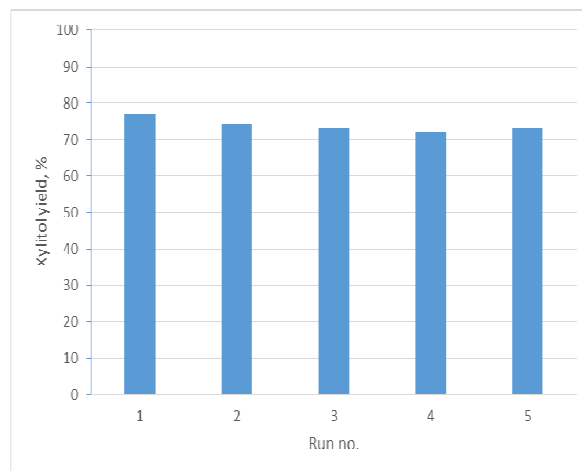
### 3.2. ICP analysis

The ICP result reveals impurities (P, N, Ru) in the xylan raw material. We calculated the amount of impurities for a typical reaction solution with 75 mg xylan, which is given below.

**Table S2:** Experimental and theoretical composition of xylan determined by ICP.

%C		%H		%N		%Ru		%P		%O	
EXP	THEO	EXP	THEO	EXP	THEO	EXP	THEO	EXP	THEO	EXP	THEO
43.07	45.45	5.53	6.12	0.05	0	0.0262	0	0.24	0	51.08	48.44

#### 4. Recycling experiments



**Figure S6.** Xylitol yield as a function of reaction time using 6 g/L of lactic acid for the hydrogenolysis reaction. Reaction conditions: xylan (0.075 g), Ru/C (0.025 g), water (8.0 ml), 160 °C, 1h, 20 bar H<sub>2</sub>.