

## Aberystwyth University

### *Production of oligosaccharides and biofuels from Miscanthus using combinatorial steam explosion and ionic liquid pretreatment*

Bhatia, Rakesh; Lad, Jai; Bosch, Maurice; Bryant, David; Leak, David; Hallett, Jason; Franco, Telma ; Gallagher, Joe

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# Supporting information

Figure.S1 FTIR spectra of untreated and pretreated *Miscanthus Mx2779*.

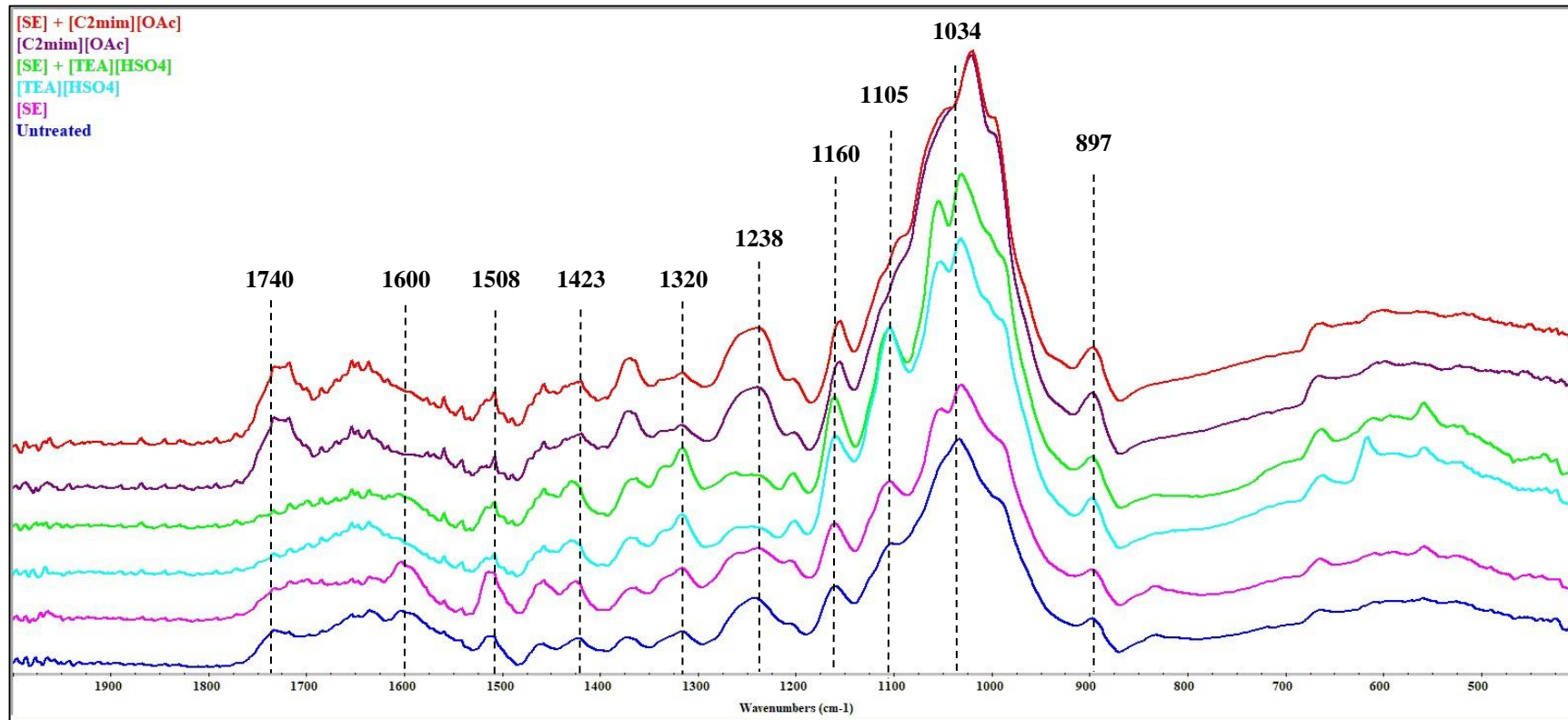


Figure S2. Gluco-oligosaccharides (GOS) and xylo-oligosaccharides (XOS) present in the liquid fraction after steam explosion and [C<sub>2</sub>mim][OAc] pretreatment of *Miscanthus Mx2779*.

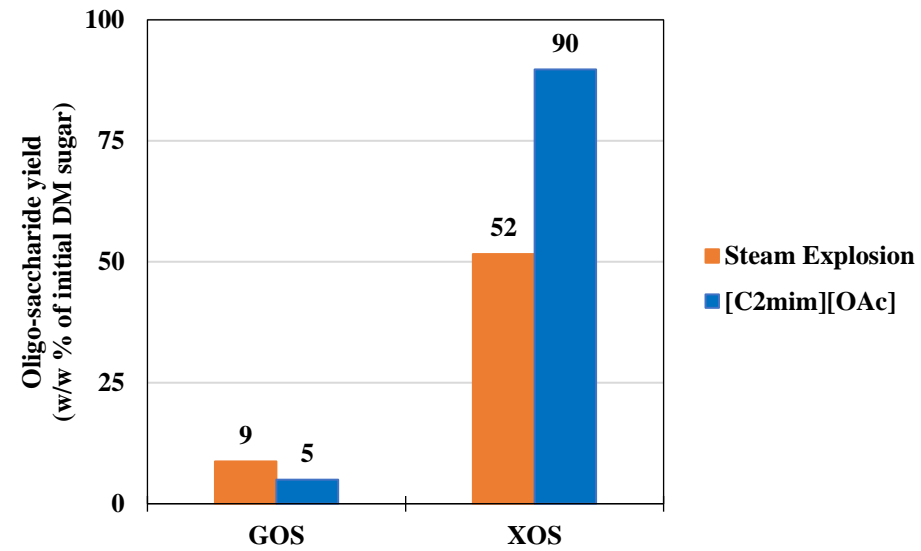


Table S1. Correlation between biomass properties and 72 hr glucan hydrolysis yields for untreated and pretreated *Miscanthus Mx2779*.

	<i>Conversion of glucan to GOS (%)</i>	<i>Xylan Content (w/w %)</i>	<i>Lignin Content (w/w %)</i>	<i>LOI (A1423/A897)</i>	<i>HBI (A3400/A1320)</i>	<i>CLL (A1508/A1600)</i>
Conversion of glucan to GOS (%)	1					
Xylan Content (w/w %)	-0.64	1				
Lignin Content (w/w %)	-0.54	0.58	1			
LOI (A1423/A897)	0.19	0.06	-0.01	1		
HBI (A3400/A1320)	0.68	-0.34	-0.72	-0.35	1	
CLL (A1508/A1600)	0.75	-0.97***	-0.53	0.09	0.32	1

A correlation coefficient of -1 indicates a perfect negative correlation. .

As xylan content decreases, CLL increases. As xylan content increases, CLL decreases.

Data are expressed as means  $\pm$  standard error (n  $\geq$  3). \* $P \leq 0.05$ ; \*\* $P \leq 0.01$ ; \*\*\* $P \leq 0.001$ .

	<i>Conversion of glucan to glucose (%)</i>	<i>Glucan Content (w/w %)</i>	<i>Xylan Content (w/w %)</i>	<i>Lignin Content (w/w %)</i>	<i>Acetyl Content (w/w %)</i>
Conversion of glucan to glucose (%)	1				
Glucan Content (w/w %)	-0.16	1			
Xylan Content (w/w %)	-0.98***	0.06	1		
Lignin Content (w/w %)	-0.61	0.49	0.58	1	
Acetyl Content (w/w %)	-0.51	-0.44	0.51	0.41	1

A correlation coefficient of -1 indicates a perfect negative correlation.

As xylan content increases, glucose yields decreases. As xylan content decreases, glucose yields increases.

Data are expressed as means  $\pm$  standard error (n  $\geq$  3). \* $P \leq 0.05$ ; \*\* $P \leq 0.01$ ; \*\*\* $P \leq 0.001$ .

	<i>Conversion of glucan to glucose (%)</i>	<i>LOI (A1423/A897)</i>	<i>HBI (A3400/A1320)</i>	<i>CLL (A1508/A1600)</i>
Conversion of glucan to glucose (%)	1			
LOI (A1423/A897)	-0.09	1		
HBI (A3400/A1320)	0.47	-0.24	1	
CLL (A1508/A1600)	0.92***	0.15	0.32	1

A correlation coefficient of 1 indicates a perfect positive correlation.

As CLL (lignin with condensed & cross-linked G-lignin subunits) content increases, glucose yields increases.

Data are expressed as means  $\pm$  standard error (n  $\geq$  3). \* $P \leq 0.05$ ; \*\* $P \leq 0.01$ ; \*\*\* $P \leq 0.001$ .

Table S2. Chemical reactions and conversions during pretreatment, enzymatic hydrolysis, fermentation and CHP steps.

Reaction	Conversion (%)				
	SE	[TEA][H <sub>2</sub> SO <sub>4</sub> ]	SE + [TEA][H <sub>2</sub> SO <sub>4</sub> ]	[C <sub>2</sub> mim][OAc]	SE + [C <sub>2</sub> mim][OAc]
Glucan (recovered in pretreated solids)	88%	85%	100%	86%	91%
Glucan → gluco-oligosaccharides (GOS)	9%	n.d	n.d	5%	bdl
Glucan + H <sub>2</sub> O → glucose	bdl	n.d	n.d	bdl	bdl
Xylan (recovered in pretreated solids)	27%	44%	53%	10%	13%
Xylan → xylo-oligosaccharides (XOS)	52%	n.d	n.d	88%	87%
Xylan + H <sub>2</sub> O → xylose	5%	n.d	n.d	bdl	bdl
Lignin → insoluble lignin	96%	36%	31%	26%	33%
Lignin → soluble lignin	4%	64%	69%	74%	67%
Acetyl → acetic acid	63%	100%	100%	42%	17%
<b>Enzymatic hydrolysis (72 hr)</b>					
Glucan → glucose (conversion factor)	1.11				
Xylan → xylose (conversion factor)	1.14				
Glucan + H <sub>2</sub> O → glucose (hydrolysis efficiency)	70%	65%	79%	93%	94%
Xylan + H <sub>2</sub> O → xylose (hydrolysis efficiency)	73%	55%	75%	63%	79%
<b>Fermentation</b>					
Glucose → EtOH (conversion factor)	0.511				
Glucose → CO <sub>2</sub> (conversion factor)	0.489				
Glucose (fermentation efficiency)	95%				
Xylose (fermentation efficiency)	70%				
EtOH (Density kg/L)	0.789				
EtOH (Recovery)	98.8%				
<b>CHP (combined heat and power)</b>					
Higher heating value of lignin post pretreatment and enzymatic hydrolysis (GJ/tonne)	21.72				
CHP (efficiency)	75%				
1 GJ (in kWh)	278				

n.d: not determined.

Bdl: below detection limit.