

## **Supporting Information**

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2013

## Simulated Moving Bed Chromatography: Separation and Recovery of Sugars and Ionic Liquid from Biomass Hydrolysates

Benjamin R. Caes, [a, b] Thomas R. Van Oosbree, [a, c] Fachuang Lu, [a, c] John Ralph, [a, c] Christos T. Maravelias, [a, d] and Ronald T. Raines\*[a, b, c]

cssc\_201300267\_sm\_miscellaneous\_information.pdf

Page	Contents
S1	Table of Contents
S2	Table S1. Dependence of [BMIM]CI recovery on its concentration
S2	Table S2. Dependence of [BMIM]CI, glucose, and xylose recovery on extract flow rate
S2	Table S3. Yield of glucose and xylose from acid hydrolysis of biomass in recycled [BMIM]CI
S3	Figure S1. Single-column separation of [BMIM]Cl and glucose.
S3	Figure S2. Adsorption isotherm of [BMIM]Cl and glucose.
S3	<b>Figure S3.</b> Representative example of an SMB chromatography parameter calculator worksheet for a three-zone configuration
S4	<b>Figure S4.</b> <sup>1</sup> H NMR spectra showing the effect of hydrolysis reaction conditions (30 days) on the integrity of [BMIM]CI.

**Table S1.** Dependence of [BMIM]CI recovery on its concentration

CONCENTIALION	
[BMIM]CI Feed	[BMIM]CI Recovery
Concentration (mg/mL)	in Raffinate (%) <sup>[a]</sup>
200	97
250	83
300	33
400	24

<sup>&</sup>lt;sup>[a]</sup>Percent recovery refers to the recovered amount relative to the loaded amount.

Table S2. Dependence of [BMIM]CI, glucose, and xylose recovery on extract flow rate

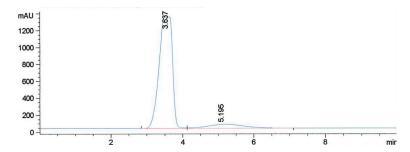
Extract Flow		Recovered	Recovered	Recovered
Rate (mL/min)	Sample	[BMIM]CI (%) <sup>[a]</sup>	Glucose (%) <sup>[a]</sup>	Xylose (%) <sup>[a]</sup>
1.3	Raffinate	98	31	13
1.3	Extract	2	69	87
1.4	Raffinate	97	27	0
1.4	Extract	3	73	100
1.5	Raffinate	89	0	0
1.5	Extract	11	100	100
1.6	Raffinate	65	0	0
1.6	Extract	35	100	100

<sup>&</sup>lt;sup>[a]</sup>Percent recovery refers to the recovered amount relative to the loaded amount.

**Table S3.** Yield of glucose and xylose from acid hydrolysis of biomass in recycled [BMIM]CI

1 8 18 66 2 8 3 5 1 12 12 40	Stage	[HCI] (M)	Glucose Molar Yield (%) <sup>[a]</sup>	Xylose Molar Yield (%) <sup>[a]</sup>
1 12 12 40	1	8	18	66
	2	8	3	5
2 12 8 12	1	12	12	40
	2	12	8	12

<sup>&</sup>lt;sup>tal</sup>Yields are based on HPLC analysis and are relative to glucose and xylose monomers in corn stover.



**Figure S1.** Single-column separation of [BMIM]CI and glucose. A mixture of [BMIM]CI and glucose was injected onto a Dowex $^{\otimes}$  50WX4-400 ion exclusion column. The column was eluted with deionized water at 2 mL/min at ambient temperature.

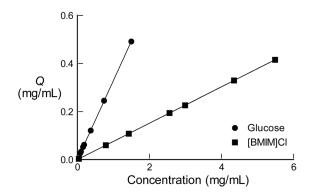


Figure S2. Adsorption isotherm of [BMIM]CI and glucose.

Dov	velonment Colun	nn Volume:	19.63	
Development Column Volume: Flow Rate for $t_0$ ml/min:			2	
Flow Rate for $t_0$ min:			3.1	
,	Void Fraction of	-0	0.32	
·		ak 1 $T_r$ min:	3.64	
		ak 2 $T_r$ min:	5.2	
		onstant <i>H</i> <sub>1</sub> :	0.08	
	•	onstant <i>H</i> <sub>2</sub> :	0.31	
	•	vity ( <i>H</i> <sub>2</sub> / <i>H</i> <sub>1</sub> ):	3.89	
		7.9		
SMBC Column Volume ml: Extra Column Volume ml:			0.39	
	Volume iii.	0.55		
Scenario:	1	2	3	4
Switch Time, sec:	40	40	40	40
Q <sub>feed</sub> ml/min:	0.25	0.25	0.25	0.25
Q <sub>desorbent</sub> ml/min:	4.5	4.5	4.5	4.5
Q <sub>extract</sub> ml/min:	1.3	1.4	1.5	1.6
Q <sub>raffinate</sub> ml/min:	3.45	3.35	3.25	3.15
Q <sub>recycle</sub> ml/min:	3.0	3.0	3.0	3.0
Q₁ ml/min:		7.50	7.50	7.50
Q₂ ml/min:	6.20	6.10	6.00	5.90
Q₃ ml/min:	6.45	6.35	6.25	6.15
Q₄ ml/min:	3.00	3.00	3.00	3.00
m <sub>1</sub> :	0.39	0.39	0.39	0.39
m <sub>2</sub> :	0.23	0.22	0.21	0.19
m <sub>3</sub> :	0.26	0.25	0.24	0.22
m <sub>4</sub> :	0.26	-0.16	-0.16	-0.16
Mass Balance, ml/min:	4.75	4.75	4.75	4.75

**Figure S3.** Representative example of an SMB chromatography parameter calculator worksheet for a three-zone configuration.

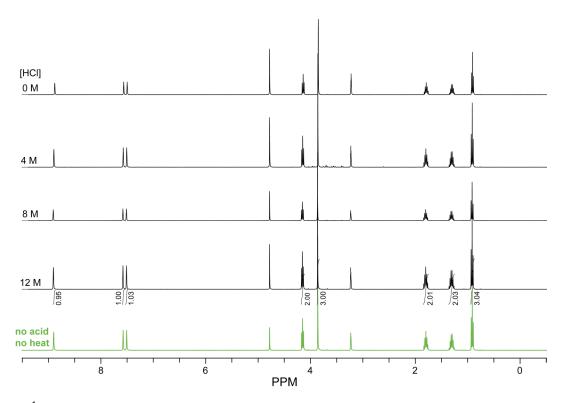


Figure S4.  $^{1}$ H NMR spectra showing the effect of a 30-day exposure to hydrolysis reaction conditions (105°C) on the integrity of [BMIM]CI.