ONE-POT ETHANOL PRODUCTION UNDER OPTIMIZED PRETREATMENT CONDITIONS USING AGAVE BAGASSE AT HIGH SOLIDS LOADING WITH LOW-COST BIOCOMPATIBLE PROTIC IONIC LIQUID

José A. Pérez-Pimienta[a,b], Gabriella Papa[c], Jian Sun[c,d], Vitalie Stavila[e], Arturo Sanchez[a], John M. Gladden[c,d], Blake A. Simmons[c,*]

[a] Laboratorio de Futuros en Bioenergía, Unidad Guadalajara de Ingeniería Avanzada, Centro de Investigación y Estudios Avanzados (CINVESTAV), Zapopan, Mexico

[b] Department of Chemical Engineering, Universidad Autónoma de Nayarit, Tepic, Mexico

[c] Joint BioEnergy Institute, Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Emeryville, CA, United States

[d] Department of Biomass Science and Conversion Technology, Sandia National Laboratories, Livermore, CA, United States

[e] Energy Nanomaterials Department, Sandia National Laboratories, Livermore, CA, United States

*Corresponding author

E-mail address: japerez@uan.edu.mx

Telephone: +52-3112118821

Table S1. ANOVA results from the response surface quadratic model for the glucan and xylan conversion for optimization of ionic liquid pretreatment using Agave bagasse.

Response	Source	df[a]	SS[b]	MS[c]	F-ratio	Sig.	R^2/adjusted R^2	CV(%)[d]/adequate precision
Glucan	Model	9	5374.03	597.11	23.74	<0.0001	0.9553/0.9150	9.13/17.37
	Lack of fit	5	235.8	47.16	14.98	0.005		
	Pure error	5	15.74	3.15				
	Residual	10	251.55	25.15				
	Total	19	5625.57	19				
Xylan	Model	9	1743.14	193.68	25.29	<0.0001	0.9579/0.9200	14.29/17.72
	Lack of fit	5	69.22	13.84	9.41	0.014		
	Pure error	5	7.36	1.47				
	Residual	10	76.57	7.66				
	Total	19	1819.71					

Calculated by using the multiple regression model:

- ❖ Glucan conversion (%) = 365.91173 - 5.04206*Temperature – 1.82364*IL concentration + 0.658486*Time + 0.002135 *Temperature*IL concentration + 0.054046* Temperature* Time - 0.009197*IL concentration*Time + 0.021504*Temp^2 + 0.012018*ILconcentration^2 - 0.26773*Time^2
- ❖ Xylan conversion (%) = 129.03587 – 2.24613*Temperature – 0.139742*IL concentration – 2.70466*Time – 0.003018*Temperature*IL concentration + 0.057846*Temperature*Time – 0.013698*IL concentration*Time + 0.010842*Temperature^2 + 0.004111*ILconcentration^2 – 0.131845*Time^2

[a]Degrees of freedom in the source

[b]Sum of squares due to the source

[c]Mean sum of squares due to the source

[d]Coefficient of variation

Table S2: Aromatic compounds detected in the untreated agave bagasse, EMAL and OP samples using Py-GC/MS.

Num	**Compounds**	**Elution Time**	**Mass Fragment**	**Formula**	**Origin**
1	guaiacol/mequinol/2-methoxyphenol	4.05	81/109/124	$C_7H_8O_2$	G
2	4-methylphenol, p-cresol		77,79,107,108	C_7H_8O	H
3	Pyrocatechol	4.3	97,140	$C_7H_8O_3$	G
4	2-methoxy-4-methyl phenol (creosol)	6.27	67,95,123,138	$C_8H_{10}O_2$	
5	4-vinyl phenol (shows 2,3-dihydro benzofuran)-coumaran	7.65	91/120	C_8H_8O	H
6	4-ethylguaiacol (4-ethyl-2methoxy phenol)	9.4	137/152	$C_9H_{12}O_2$	G
7	4-vinylguaiacol (2-methoxy-4 vinyl phenol)	11.08	77/107/135/150	$C_9H_{10}O_2$	G
9	2,6-dimethoxy phenol/syringol	12.82	65/93/ 139/154	$C_8H_{10}O_3$	S
10	phenol, 2 methoxy-5-(2propenyl) 3-allyl-6-methoxyphenol	1.95	65/77/91/103/131/154/164	$C_{10}H_{12}0_2$	G
11	isovanillin/p-arisaldehyde	13.7 14.15	151/152	$C_8H_8O_3$	G
12	Phenol 2, methoxy-5 (1 propenyl)	14.23	77/91/ 103/ 164	$C_1OH_1I_{22}$	G
13	4-methoxy-3-methoxymethyl phenol	15.04	168	$C_9H_{12}O3$	G
14	4-propenyl guaiacol (2-methoxy-4-propenyl phenol) isoeugenol	15.19	77/ 91/103/164	$C_{10}H_{12}O_2$	G
15	vanillic acid	15-06	77/79/107/125/ 153/168	C_8H_8O4	G
16	4 hydroxy-3-methoxyphenylpropane Phenol 2, methoxy-4 propyl	15.3	137	$C_{10}H_{14}O_2$	G
17	p-Ethylguaiacol	16.2	137	$C_9H_{12}O2$	G
18	phenol, 4-(3-hydroxy-1propenyl-2methoxy	16.5	77/91/137/180	$C_{10}H_{12}O_3$	G
19	3-tert-butyl-4-hydroxyarisole	17.1	91/137/165/180	$C_{11}H_{16}O_2$	G
20	phenol, 2,6 dimethoxy-4-(2-propenyl) (4-allyl-2,6-dimethoxy phenol)	17.64, 18.34, 19.03	91/194	$C_{12}H_{14}O_3$	S
21	Acetosyringone (4-hydroxy-3,5-dimethoxy acetophenone)	19.43	153/181/196	$C_{10}H_{12}O_4$	S

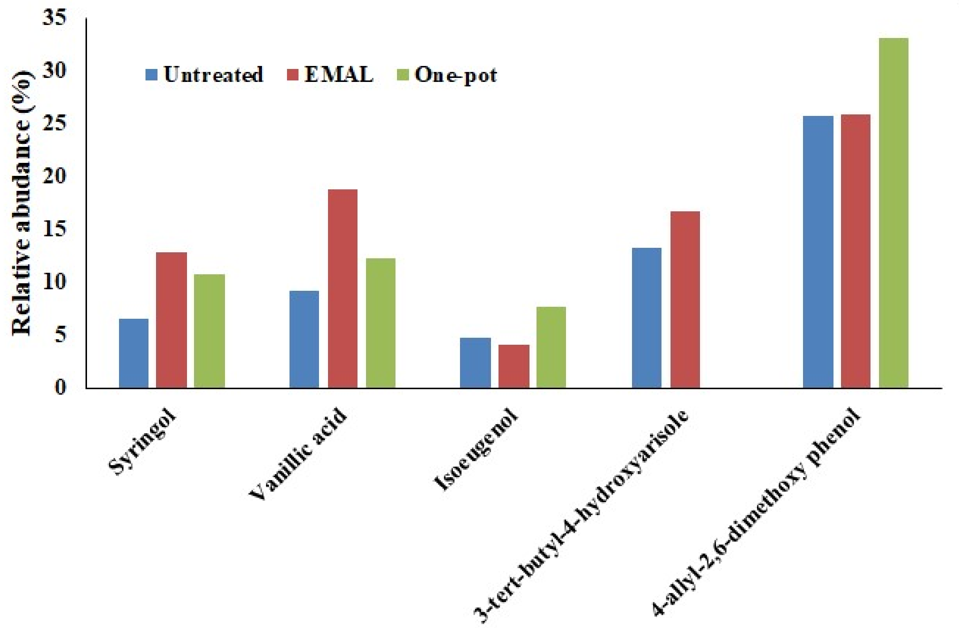

Figure S1. Relative abundance (%) of the main aromatic components detected by Py-GC/MS of untreated, EMAL and one-pot agave bagasse