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Supplementary Information

Synthesis of 1,2,3-Triazolium-Based Ionic Liquid and Preliminary Pretreatment to Enhance Hydrolysis of Sugarcane Bagasse

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Sugarcane bagasse employed

Bagasse was kindly provided by Centro de Tecnologia Canavieira, São Paulo, Brazil.

Synthesis of azidoacetic acid 5 and synthesis of azidopropan-1-ol 6

Synthesis of Azidoacetic Acid 5

To a solution of sodium azide (8.2 g, 126 mmol, 2 equiv.) in 42 mL of water bromoacetic acid **2** (10 g, 63 mmol, 1 equiv) was slowly added. The solution was stirred at room temperature overnight. The reaction mixture was acidified to pH 1 by the addition of concentrated HCl, and subsequently extracted with Et_2O (3 × 75 mL). The combined organic phases were dried over Na_2SO_4 and concentrated in vacuo to afford azidoacetic **5** acid as an oil (59 mmol, 95% yield).

Synthesis of Azidopropan-1-ol 6

To a solution of sodium azide (14.3 g, 0.216 mol, 3 equiv.) in 90 mL of DMF, 3-bromo-propan-1ol **3** (10 g, 0.072 mol, 1 equiv) was slowly added. The solution was stirred at 80 °C overnight. The reaction was monitored for the disappearance of starting materials by TLC (8:2 hexane/EtOAc) and subsequently extracted with CH_2Cl_2. The combined organic phases were dried over Na_2SO_4 and concentrated in vacuo to afford 3-azidopropan-1-ol **6** as an oil (0.065 mol, 90% yield).

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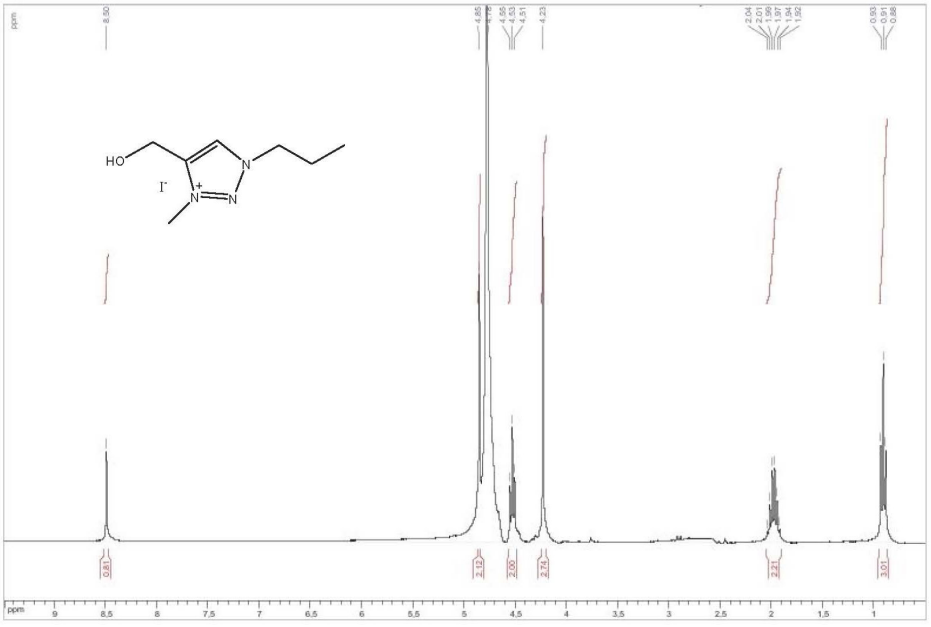


Figure S1. ^{1}H NMR spectrum (300 MHz, D_2O) of compound **10**.

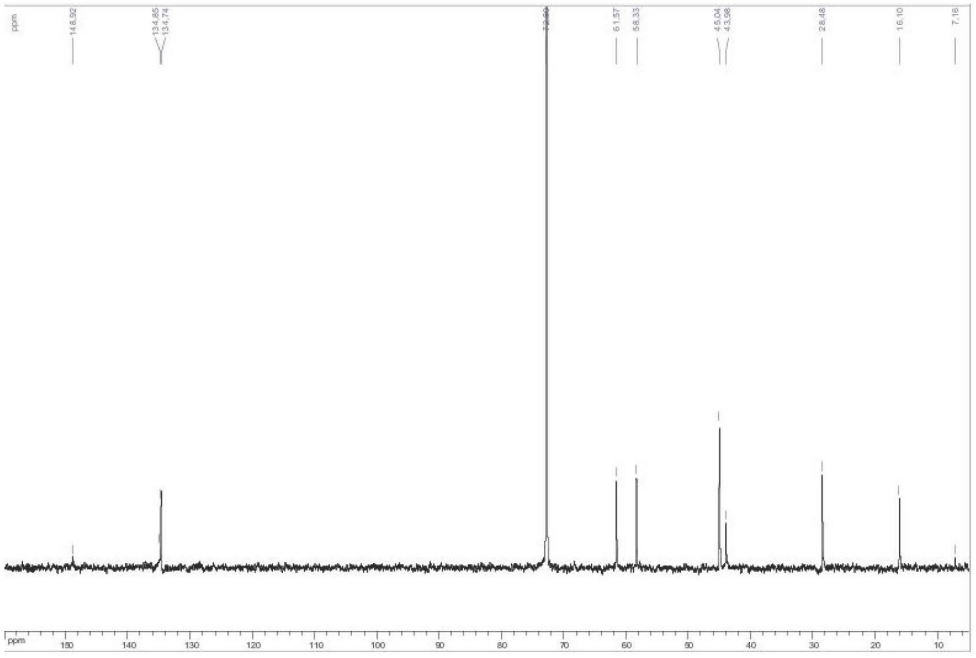
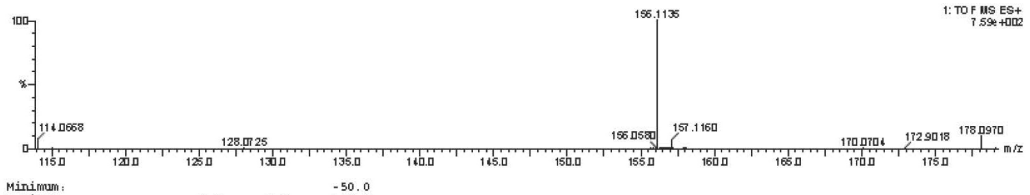


Figure S2. ^{13}C NMR spectrum (75 MHz, D_2O + dioxane) compound **10**.



Minimum:				-50.0		
Maximum:		5.0	5.0	150.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
156.1135	156.1137	-0.2	-1.3	2.5	n/a	C7 H14 N3 O

Figure S3. HRMS (MS-TOF ES+) of compound **10**.

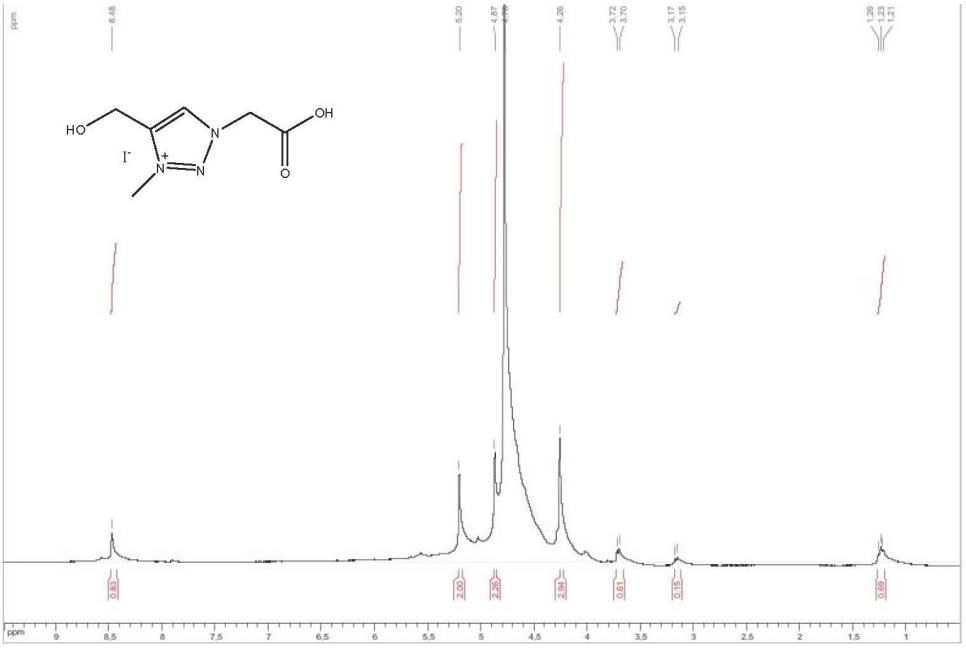


Figure S4. ^{1}H NMR spectrum (300 MHz, D_2O) of compound **11**.

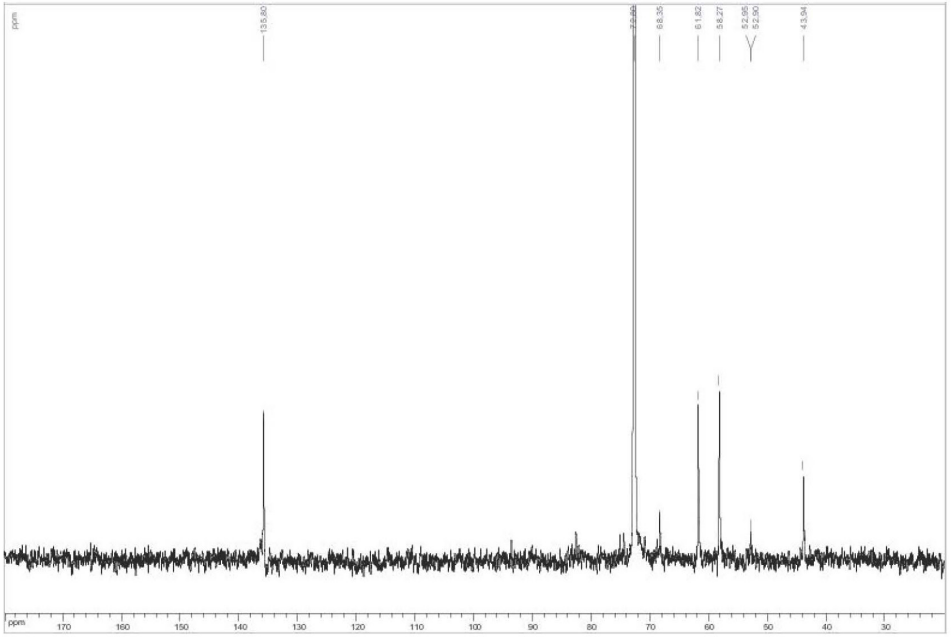
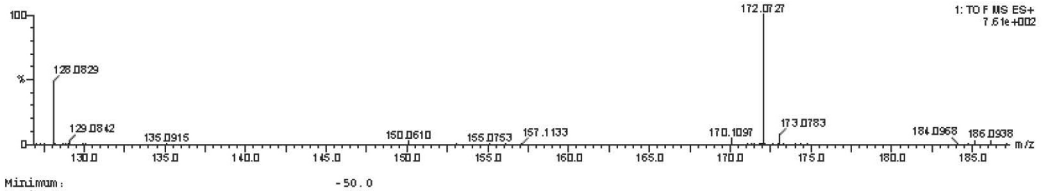


Figure S5. ^{13}C NMR spectrum (75 MHz, D_2O + dioxane) of compound **11**.



Minimum:		5.0	5.0	-50.0		
Maximum:				150.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
172.0727	172.0722	0.5	2.9	3.5	5.5	C6 H10 N3 O3

Figure S6. HRMS (MS-TOF ES+) of compound **11**.

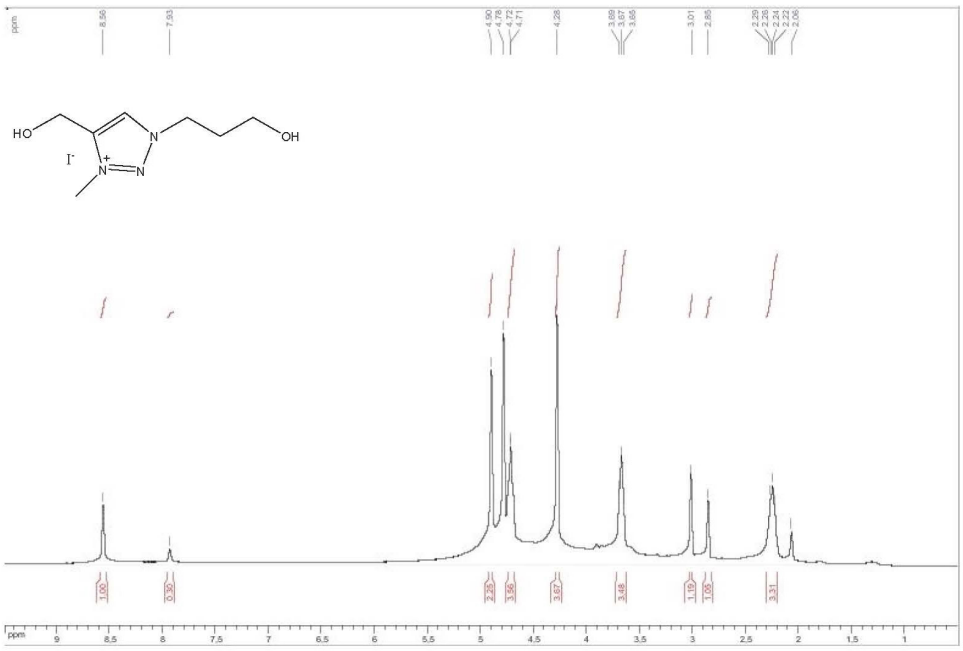


Figure S7. ^{1}H NMR spectrum (300 MHz, D_2O) of compound **12**.

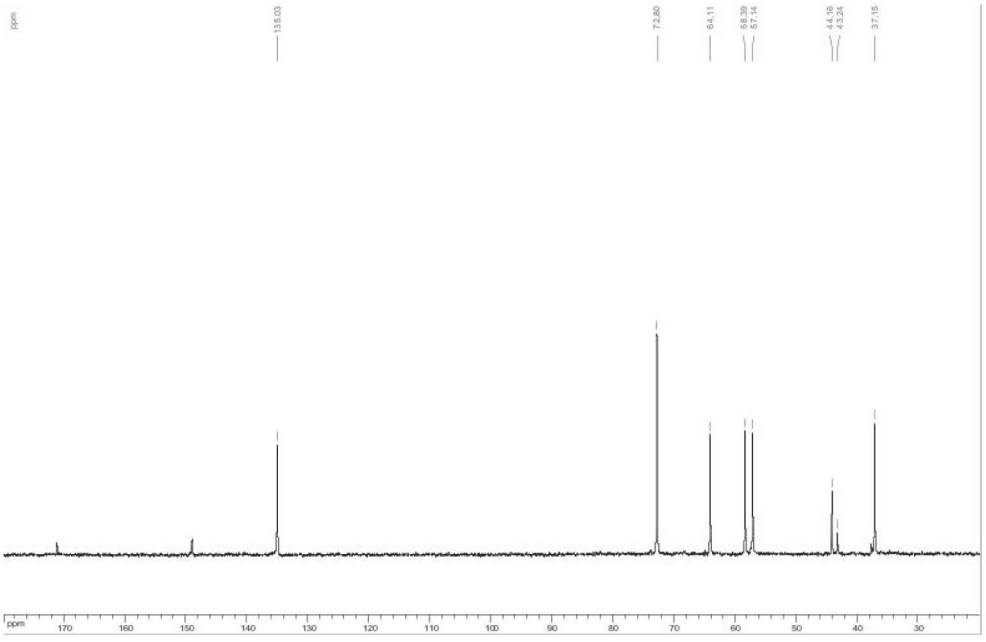
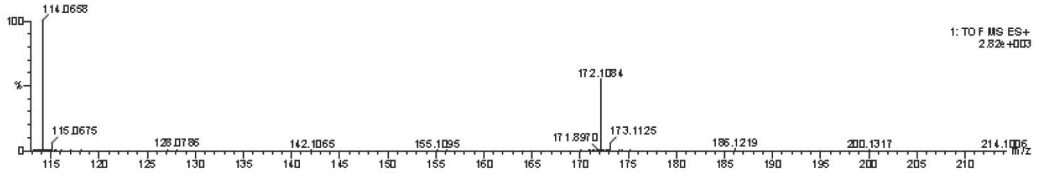


Figure S8. ^{13}C NMR spectrum (75 MHz, D_2O + dioxane) of compound **12**.



Minimum:				-50.0		
Maximum:		5.0	5.0	150.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
172.1084	172.1086	-0.2	-1.2	2.5	1.5	C7 H14 N3 O2

Figure S9. HRMS (MS-TOF ES+) of compound **12**.