Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic supplementary information

Ethanolysis of selected carbohydrates catalyzed by functionalized acidic ionic liquids: An unexpected effect of ILs structural functionalization on selectivity phenomena

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1. NMR and FT-IR spectra of synthesized ionic liquids

[bmim]HSO_4, Yield 93.1%, IR (neat): 3275, ^{1}H-NMR (200 MHz, D_2O): δ (ppm) 9.06 (s. 1H) 7.79 (s, 1H), 7.74 (s,1H), 4.18 (m, 2H), 3.76 (2, 3H), 1.75 (m, 2H), 1.25 (m, 2H), 0.91 (t, 3H); ^{13}C-NMR (120 MHz, D_2O): δ (ppm) 137.14, 126.2, 123.6, 47.60, 32.77, 34.42, 19.59, 13.47; MS (ESI-M^+) m/z 83 [HIm^+] (20%), 127.0 [M^+] (100%).

[hemim]HSO_4.Yield 92.6%, IR (neat): 3277, 3241(OH).^{1}H-NMR (200 MHz, D_2O): δ (ppm) 8.64 (s, 1H); 7.40 (s, 1H); 7.35(s, 1H); 4.19 (m, 2H); 3.79 (m, 2H); 3.78 (s, 3H),^{13}C-NMR (120 MHz, D_2O): δ (ppm) 136.4, 123.6, 122.4, 59.8, 51.1, 35.8; MS (ESI-M^+) 127.0 [M^+] (100%).

[hpmim]HSO_4.Yield 91.7%, IR (neat): 3276, 3241 (OH),^{1}H-NMR (200 MHz, D_2O): δ (ppm) 8.65 (s, 1H); 7.49 (s, 1H); 7.43 (s, 1H), 4.20 (dd, 1H), 4.02 (dd, 1H); 3.98; 3.80 (s, 3H), 3.49 (m, 2H); 1.91 (m, 2H),^{13}C-NMR (120 MHz, D_2O): δ (ppm) 136.8, 123.2, 122.5, 58.2, 48.9, 36.6, 31.5; MS (ESI-M^+) m/z 83 [HIm^+] (9%), 147.1 [M^+] (100%)

[glymim]HSO_4.Yield 92.3%, IR (neat): 3275, 3238 (OH),^{1}H-NMR (200 MHz, D_2O): δ (ppm) 8.77 (s, 1H), 7.48 (s, 1H); 7.43 (s, 1H);4.28 (dd, 2H); 4.01 (m, 1H); 3.91; 3.94; 3.89 (s, 3H); 3.61 (m, 2H),^{13}C-NMR (120 MHz, D_2O): δ (ppm) 137.3, 123.2, 123.1, 69.8, 62.4, 51.7, 35.7; MS (ESI-M^+) m/z 83 [HIm^+](41%), 157.1 [M^+] (100%)

[bmmim]HSO_4, Yield 92.8%, IR (neat): 3277, ^{1}H-NMR (200 MHz, D_2O): δ (ppm) 7.78 (d, 1H); 7.51 (d, 1H); 4.19 (m, 2H); 4.00 (a, 3H); 2.77 (s, 3H), 1.76 (m, 2H), 1.35 (m, 2H), 0.92 (t, 3H); ^{13}C-NMR (120 MHz, D_2O): δ (ppm) 145.42, 123.45, 212.95, 49.00, 35.87, 32.39, 20.16, 13.84, 10.30; MS (ESI-M^+) m/z 83 [HIm^+] (30%), 141.0 [M^+] (100%).

2. GC/MS spectra of the representative products of ethanolysis

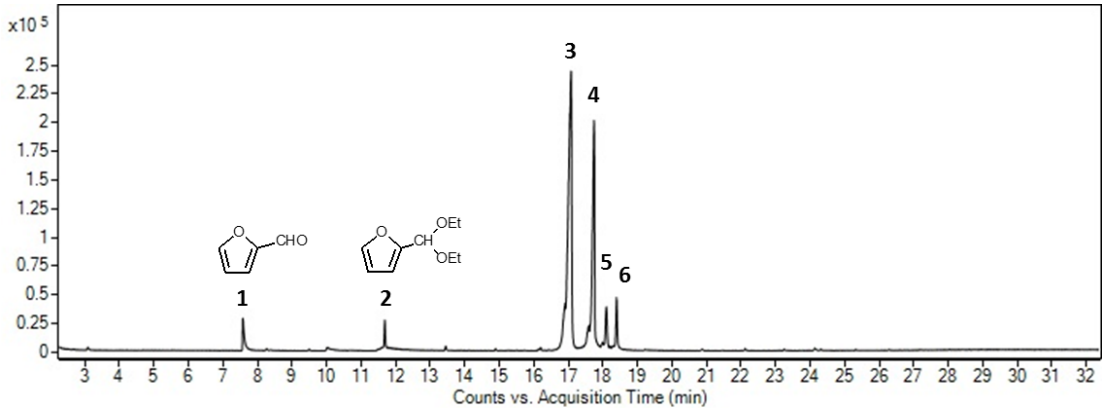

Fig. S1. GC chromatogram of the reaction product of xylose with ethanol

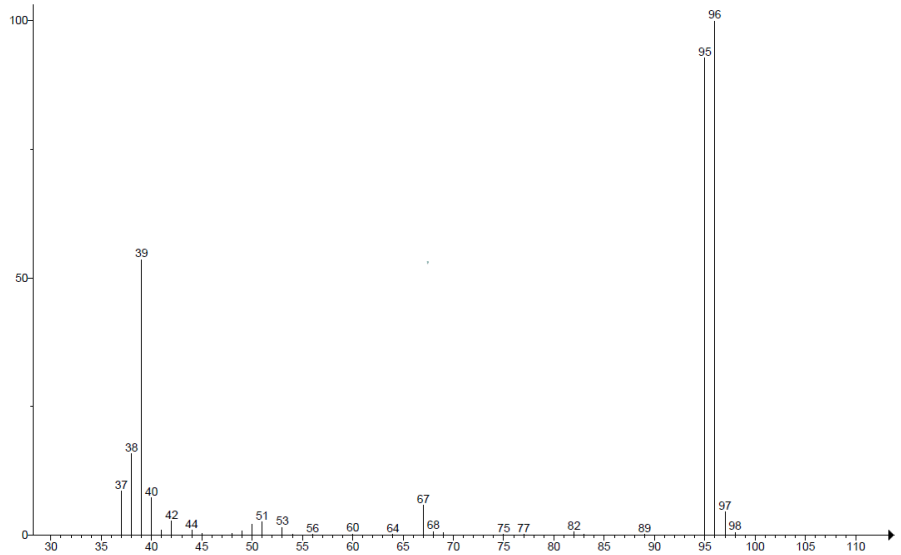

Fig. S2. MS spectrum of component **1** (τ = 7.58 min.)

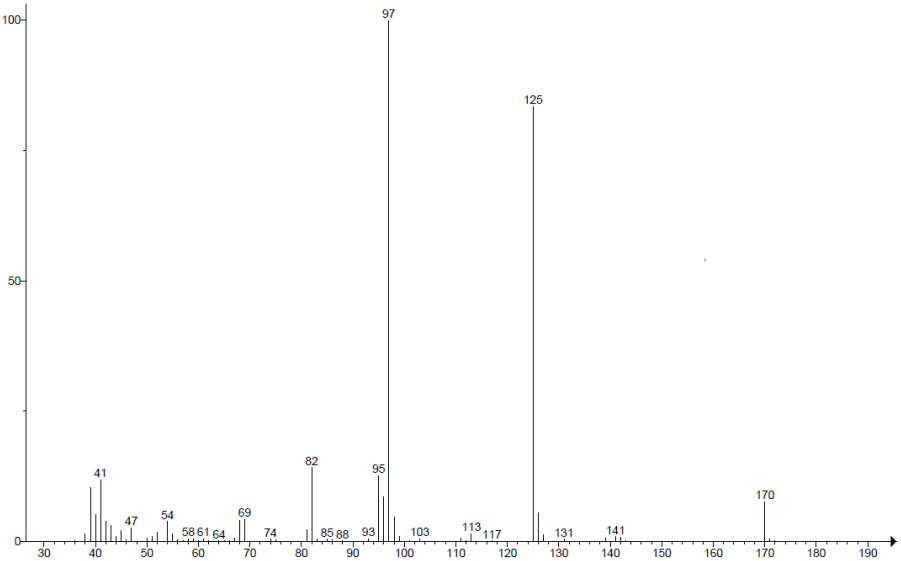

Fig. S3. MS spectrum of component **2** (11.68 min.)

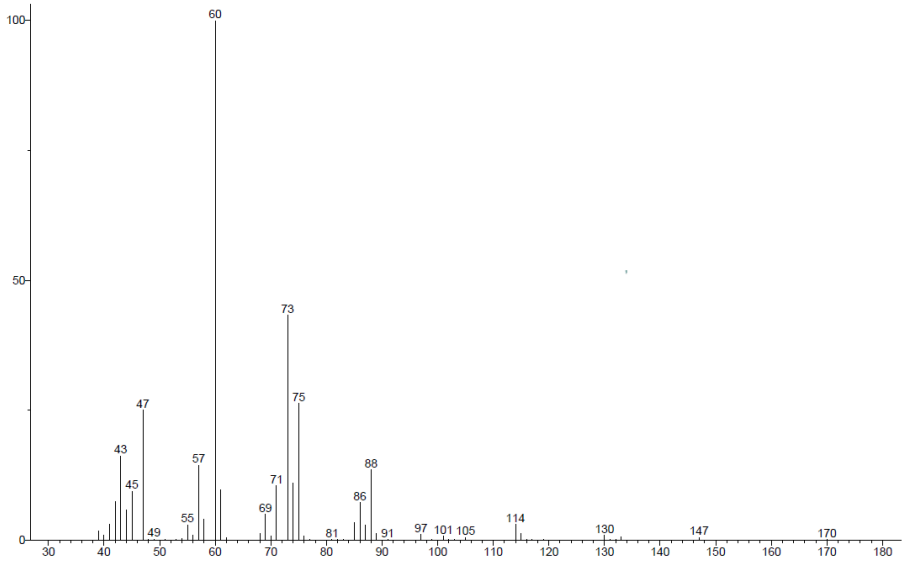

Fig. S4. MS spectrum of component 3 (τ = 17.04 min.)

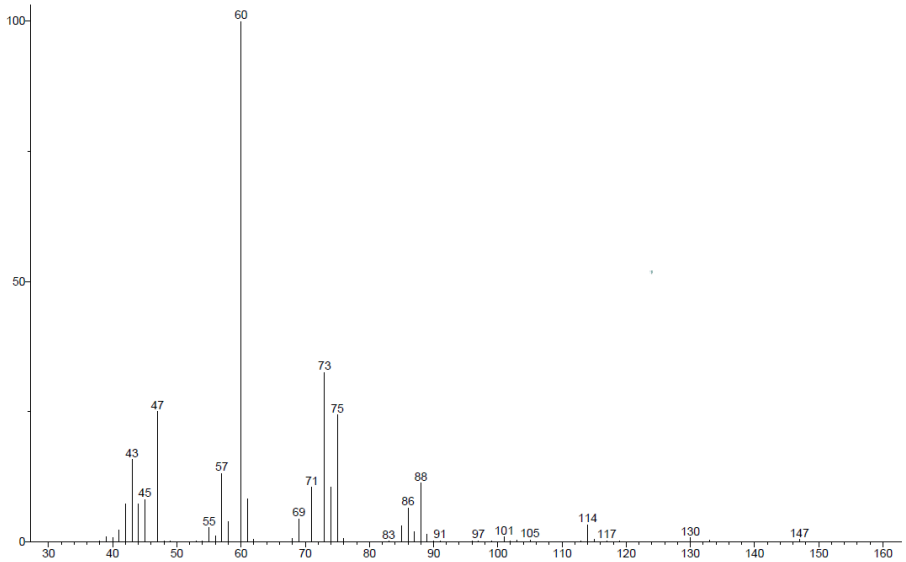

Fig. S5. MS spectrum of component 4 (τ = 17.73 min.)

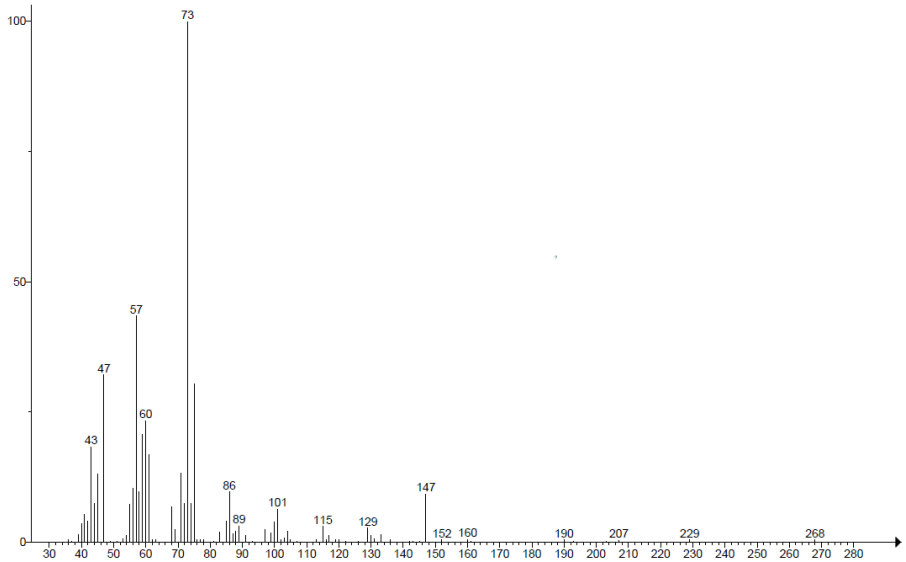

Fig. S6. MS spectrum of component **5** (τ = 18.09 min.)

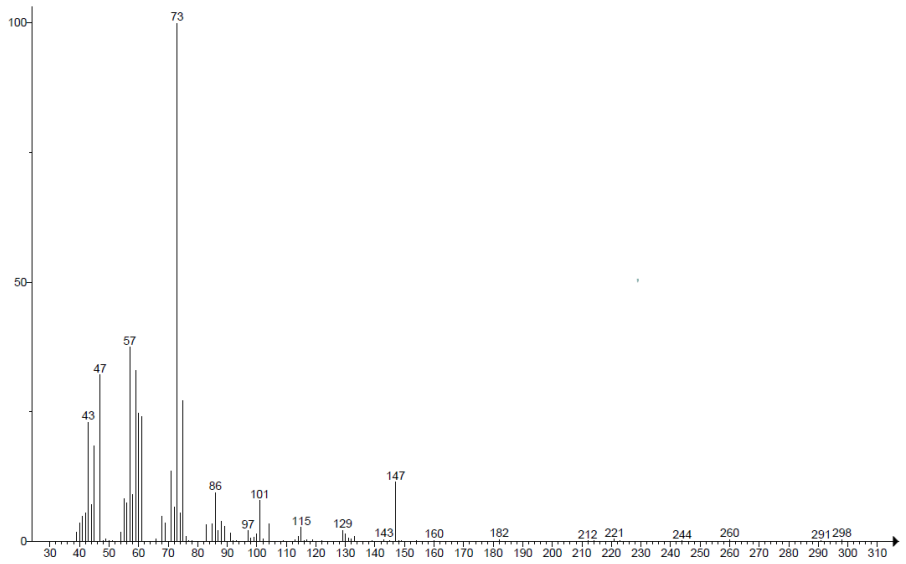

Fig. S7. MS spectrum of component **6** (τ = 18.40 min.)

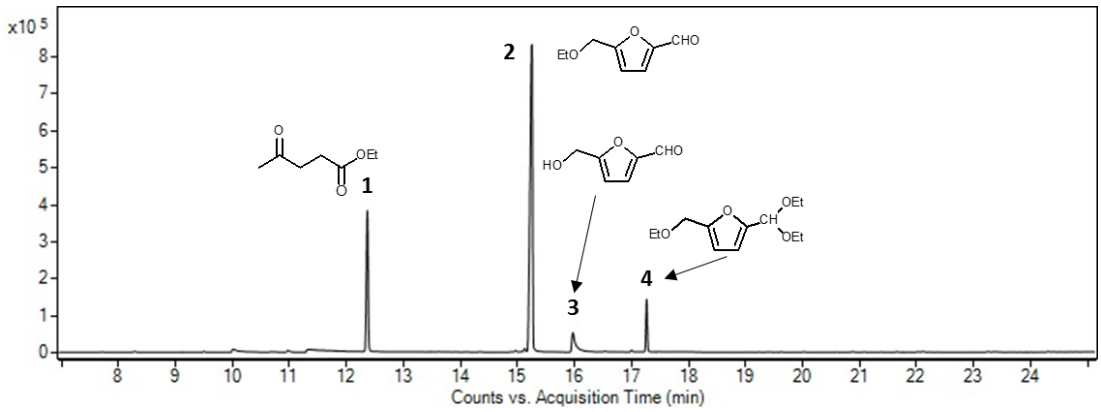

Fig. S8. GC chromatogram of the reaction product of fructose with ethanol

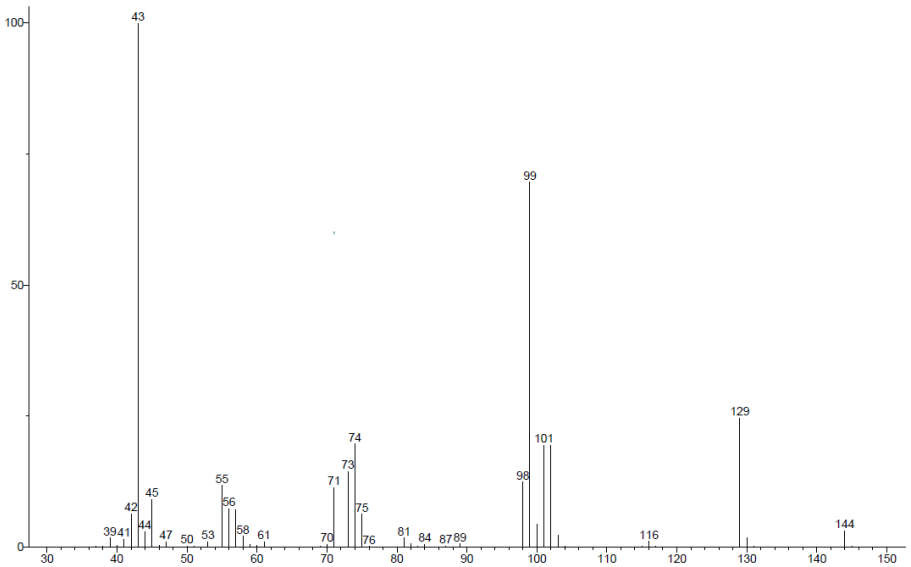

Fig. S9. MS spectrum of component **1** (ethyl levulinate), τ = 12.36 min.

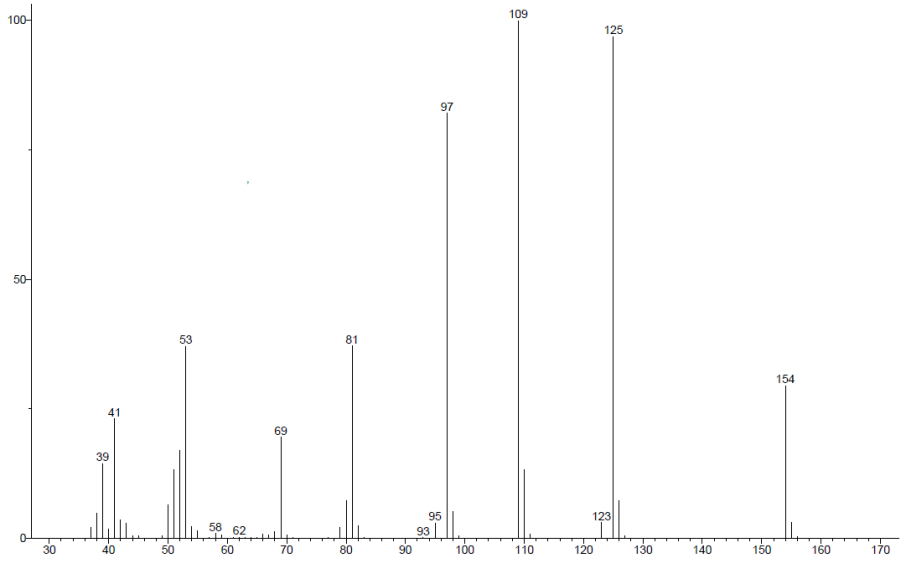

Fig. S10. MS spectrum of component **2** (5-ethoxyfuraldehyde), τ = 15.27 min.

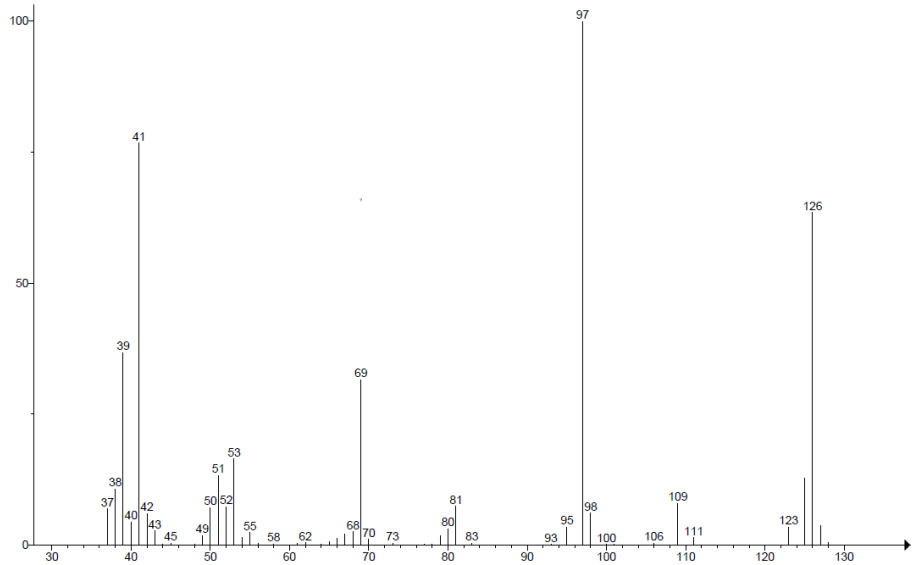

Fig. S11. MS spectrum of component **3** (5-hydroxymethylfurfural), τ = 15.97 min.

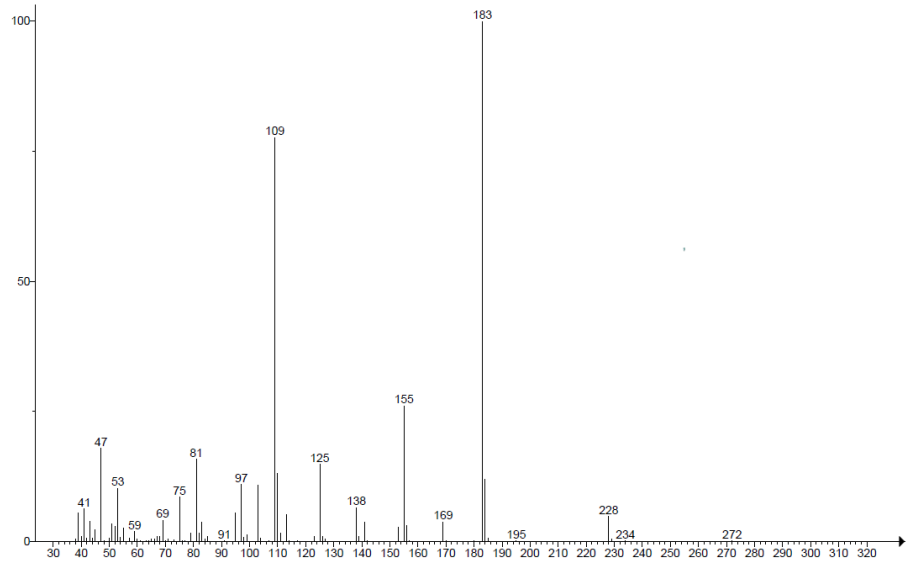

Fig. S12. MS spectrum of component **4** (diethylacetal 5-ethoxyfuraldehyde), τ = 17.26 min.

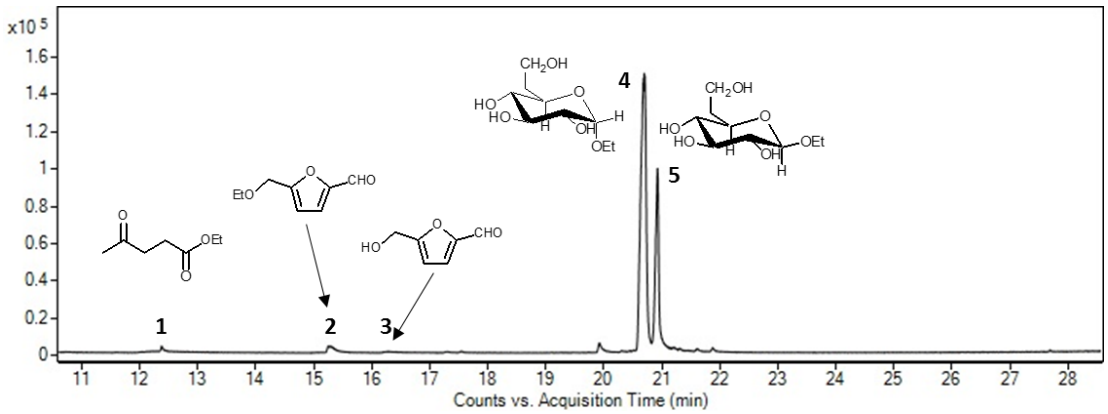

Fig. S13. GC chromatogram of the reaction product of glucose with ethanol

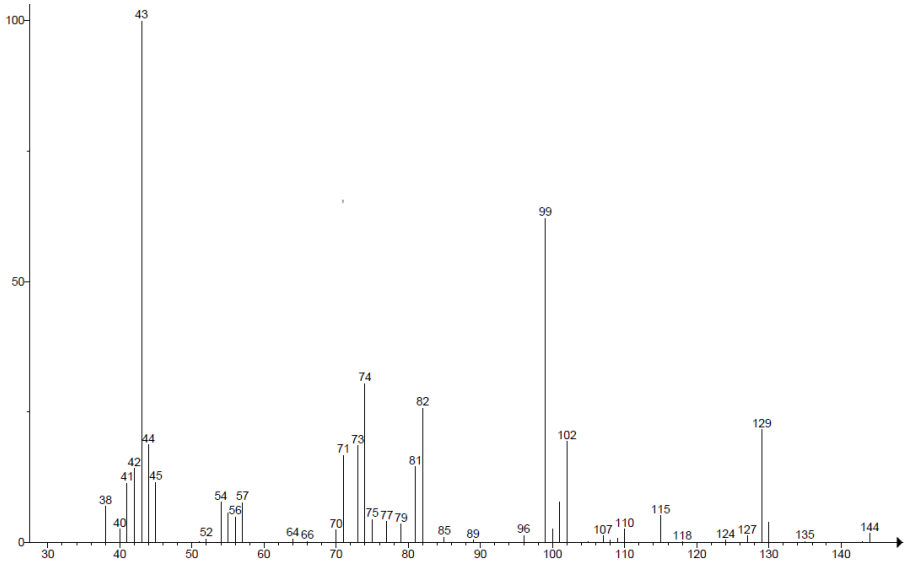

Fig. S14. MS spectrum of component **1** (ethyl levulinate), τ = 12.28

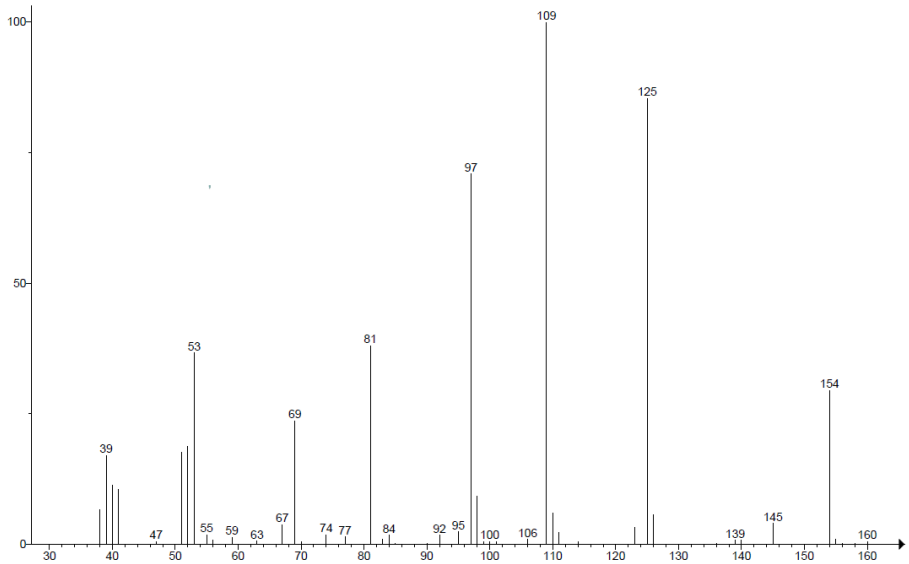

Fig. S15. MS spectrum of component **2** (5-ethoxyfuraldehyde), τ = 15.27

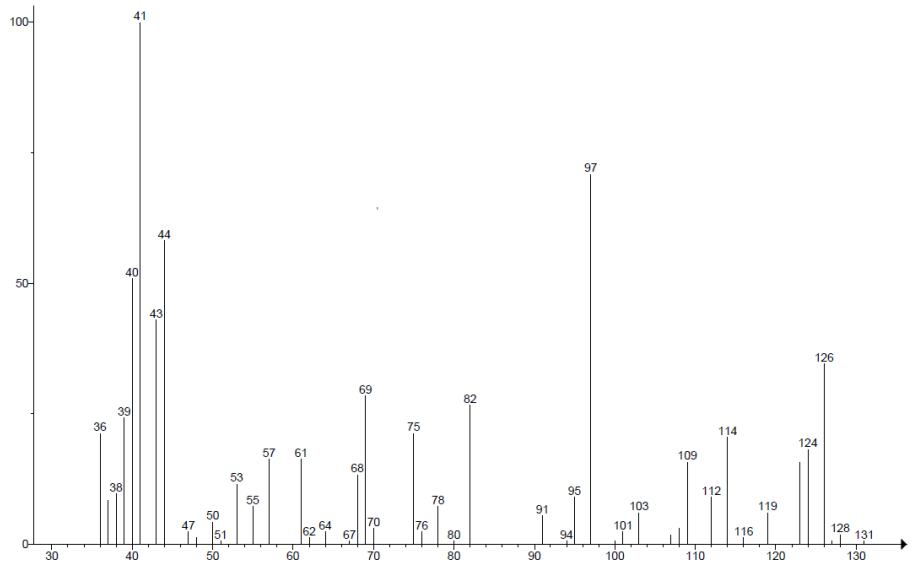

Fig. S16. MS spectrum of component **3** (5-hydroxymethylfurfural), τ = 16.28 min.

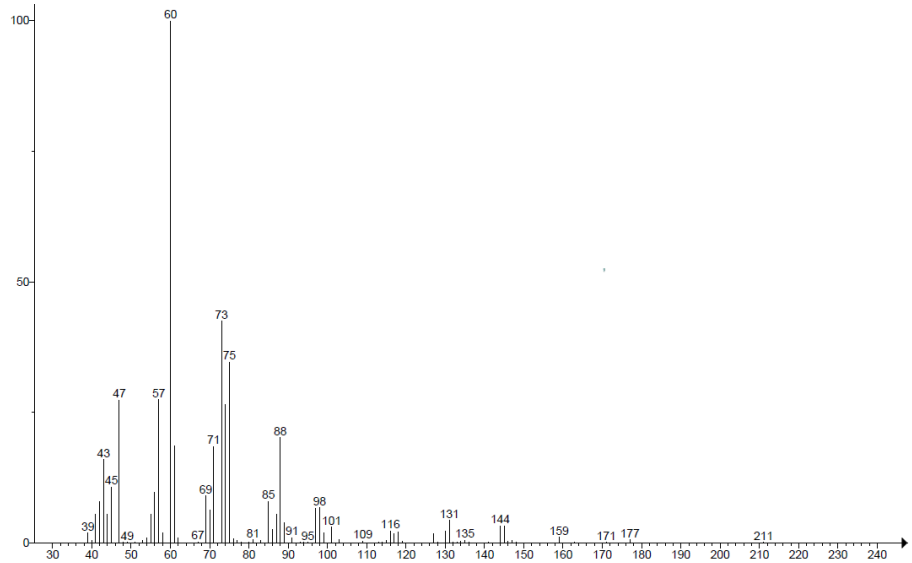

Fig. S17. MS spectrum of component **4** (ethyl α-glucopyranoside), τ = 20.69 min.

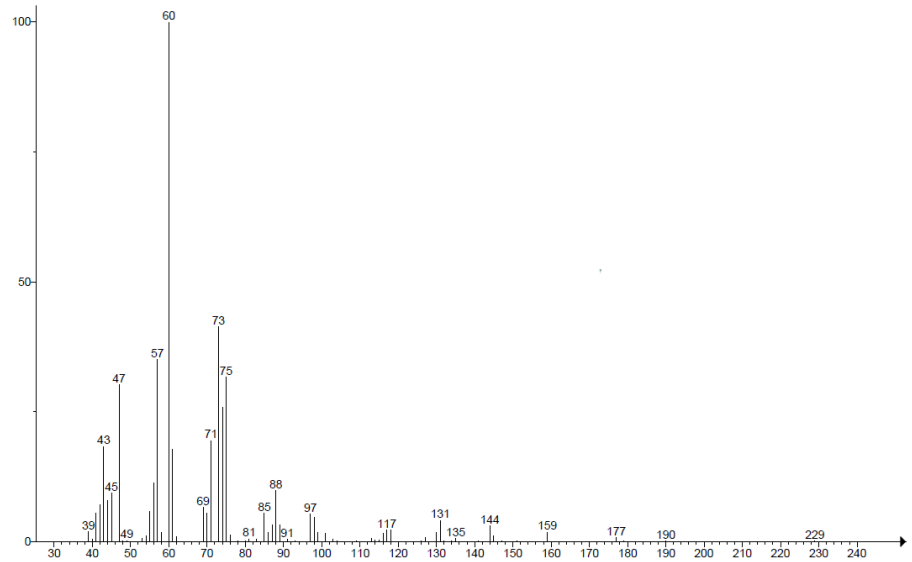

Fig. S18. MS spectrum of component **5** (ethyl β-glucopyranoside), τ = 20.93 min.