

AQUIVION® Perfluorosulfonic acid resin for butyl levulinate production from furfuryl alcohol

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Supplementary material for New Journal of Chemistry

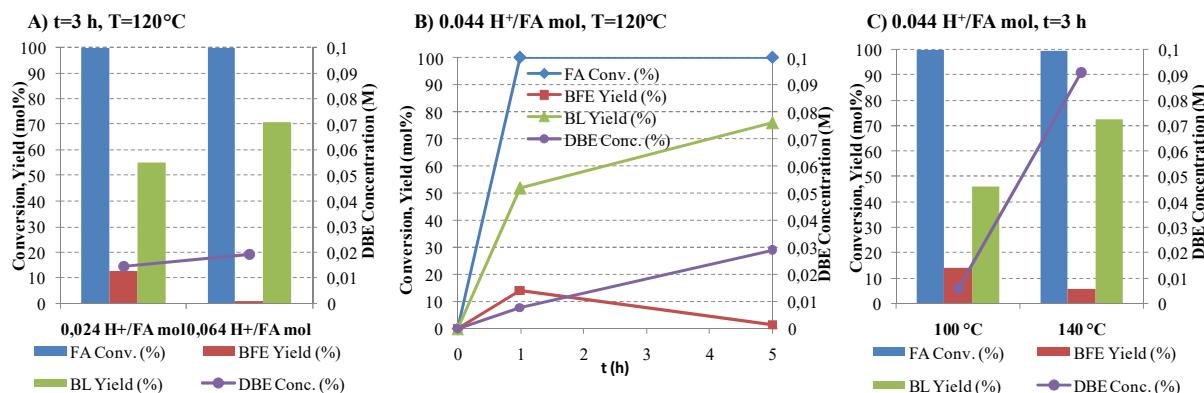


Figure S1. Main effects of each variable on FA alcoholysis. Varying A) catalyst to substrate ratio, B) time and C) temperature.

Table S1. Significance of regression coefficients for BL yield

Source	Sum of squares	degrees of freedom	Mean squares	F value	p value
x ₁	1159,331	1	1159,3	44,242	0,00029
x ₂	1272,131	1	1272,1	48,55	0,000253
x ₃	1307,501	1	1307,5	49,90	0,00022
x ₁ x ₂	29,47874	1	29,479	1,12	0,32507
x ₁ x ₃	85,60512	1	85,605	3,27	0,1135
x ₂ x ₃	151,2874	1	151,29	5,7734	0,04727
x ₁ ²	92,24772	1	92,248	3,5203	0,10273
x ₂ ²	63,91167	1	63,912	2,439	0,16232
x ₃ ²	241,1365	1	241,14	9,2021	0,01902

Table S2. ANOVA for BL yield

Source	Sum of squares	degrees of freedom	Mean squares	F value	p value
Total	5352,74	17			
Model	5169,31	9	574,37	21,92	.000253
Residuals	183,43	7	26,20		
Lack of fit	176,39	5	35,28	10,01	.093285
Pure error	7,05	2	3,52		
R ² =	0,97				
R ² _{adj} =	0,92				

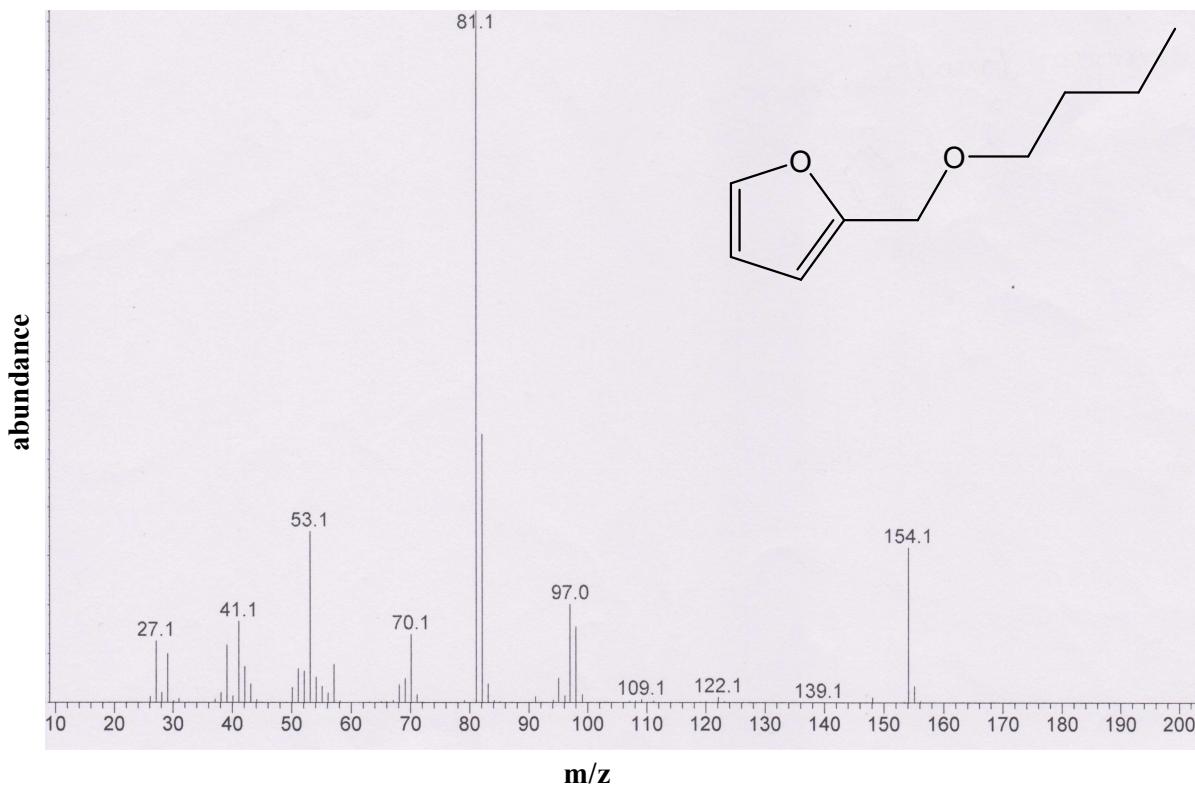


Figure S2. Mass spectra of buoxy methyl furan ether (BFE) intermediate detected by GC-MS during FA butanolysis in presence of Aquivion P87S.

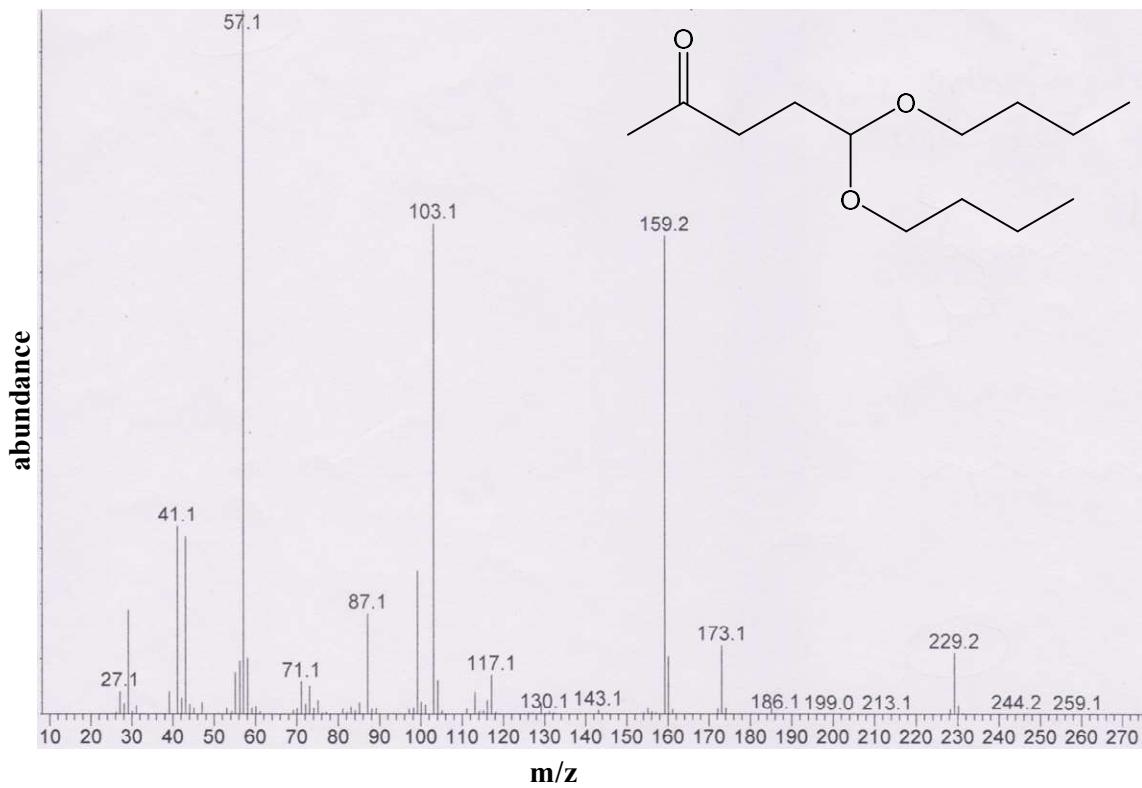


Figure S3. Mass spectra of 5,5-dibutoxy-2-pentanone (DBP) intermediate detected by GC-MS during FA butanolysis in presence of Aquivion P87S.

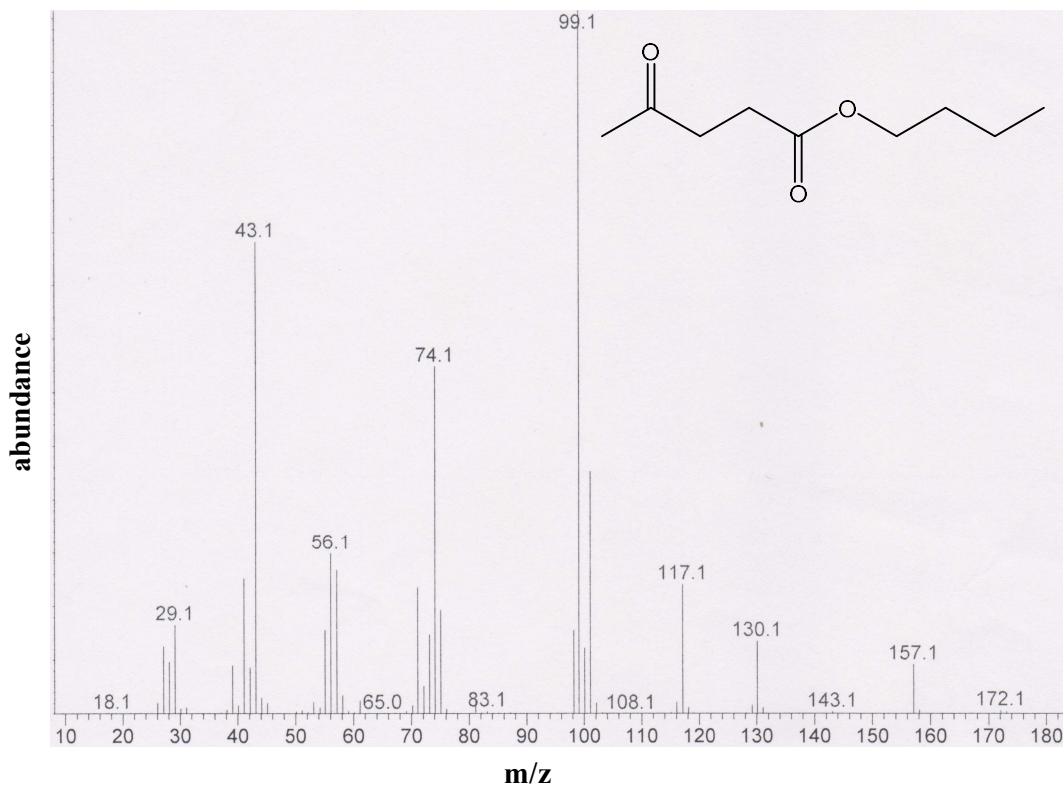


Figure S4. Mass spectra of butyl levulinate (BL) detected by GC-MS during FA butanolysis in presence of Aquivion P87S.

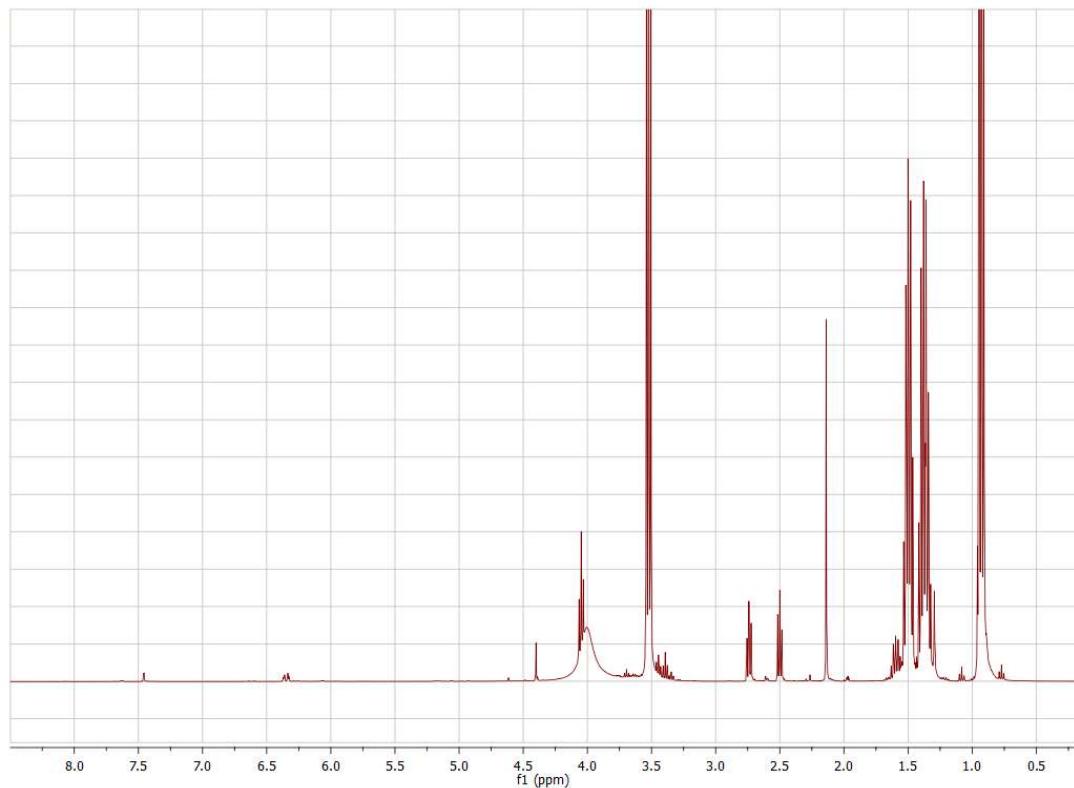


Figure S5. ^1H NMR spectrum of BL concentrated solution (13 wt.%) in CD_3CN , obtained by the semibatch operating mode.

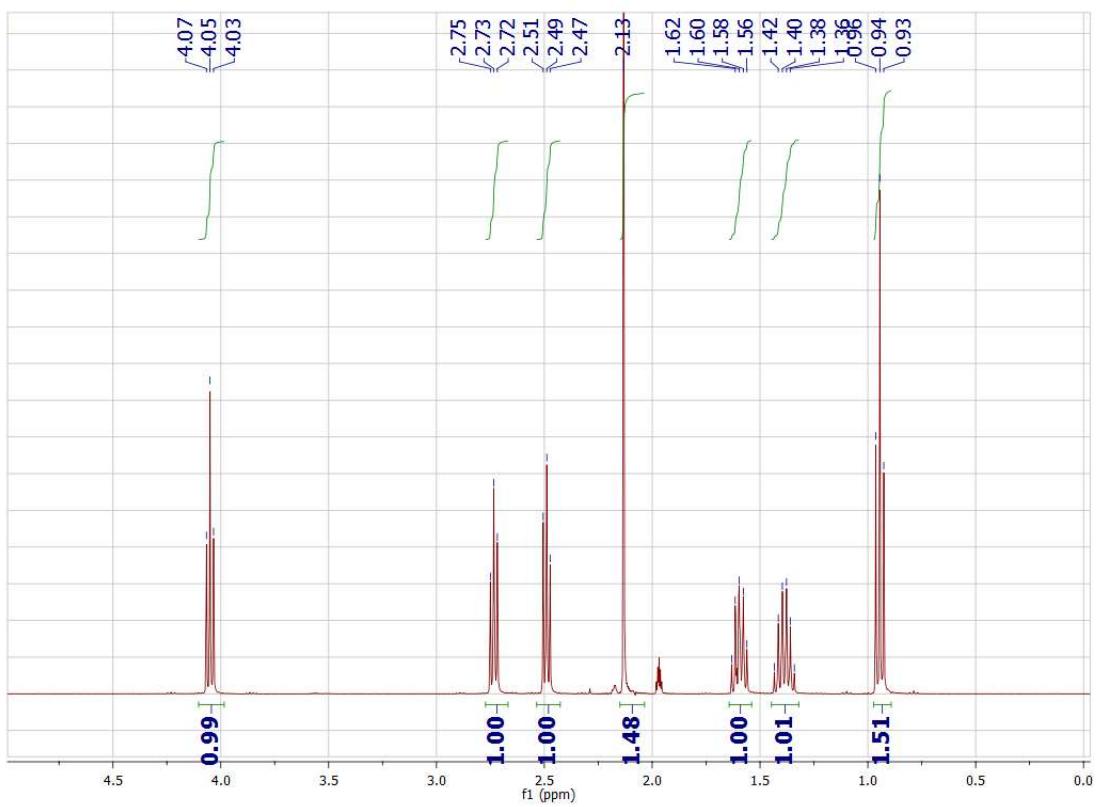


Figure S6. ^1H NMR spectrum of isolated BL in CD_3CN .

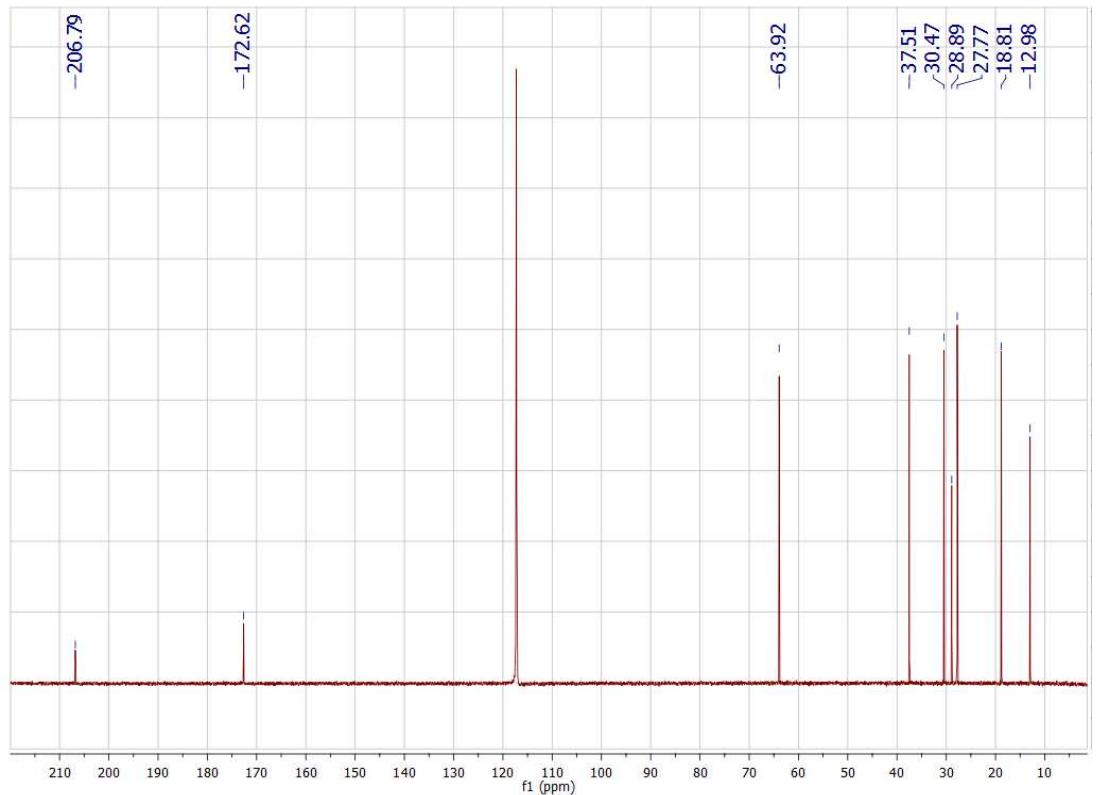


Figure S7. ^{13}C NMR spectrum of isolated BL in CD_3CN .