

## Supplementary Information

### Selective production of 1,3-butadiene using glucose fermentation liquor

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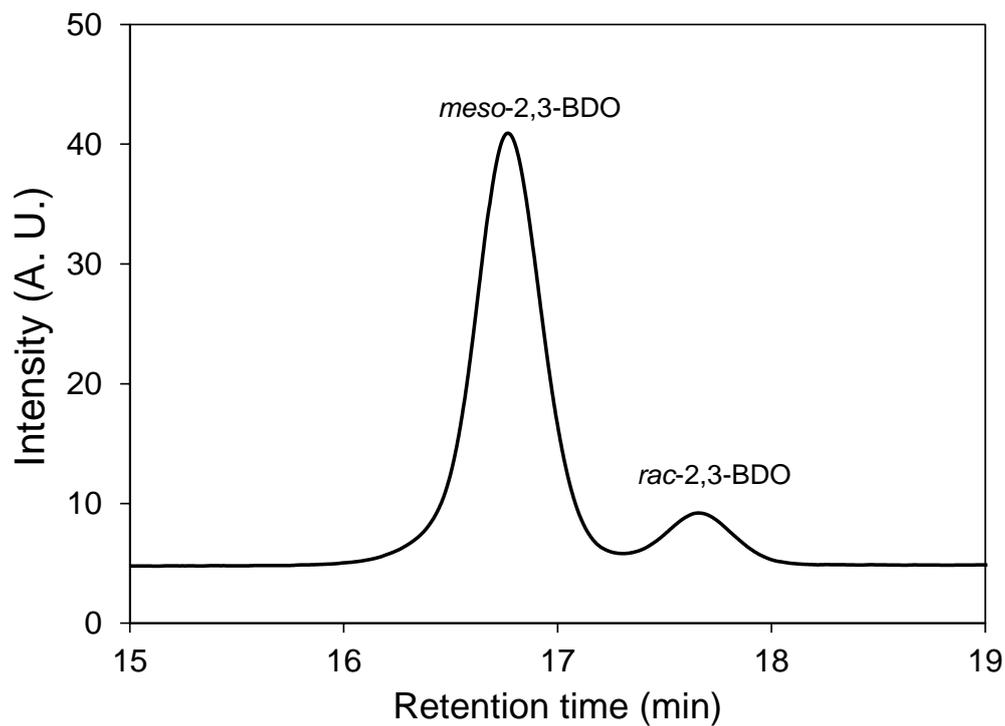
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➤ Isomer ratio of 2,3-butanediol



**Fig. S1** HPLC chromatogram of used 2,3-butanediol (Menix international corporation, >97 % purity). The molar ratio between *meso* and *racemic* 2,3-butanediol is determined to be 9 : 1 which corresponds to the ratio of 2,3-butanediol derived from glucose fermentation by *Klebsiella oxytoca* KCTC12133BP (Korean Collection for Type Cultures, Daejeon, Korea).<sup>15</sup>

➤ NMR spectra of 2,3-butanediol

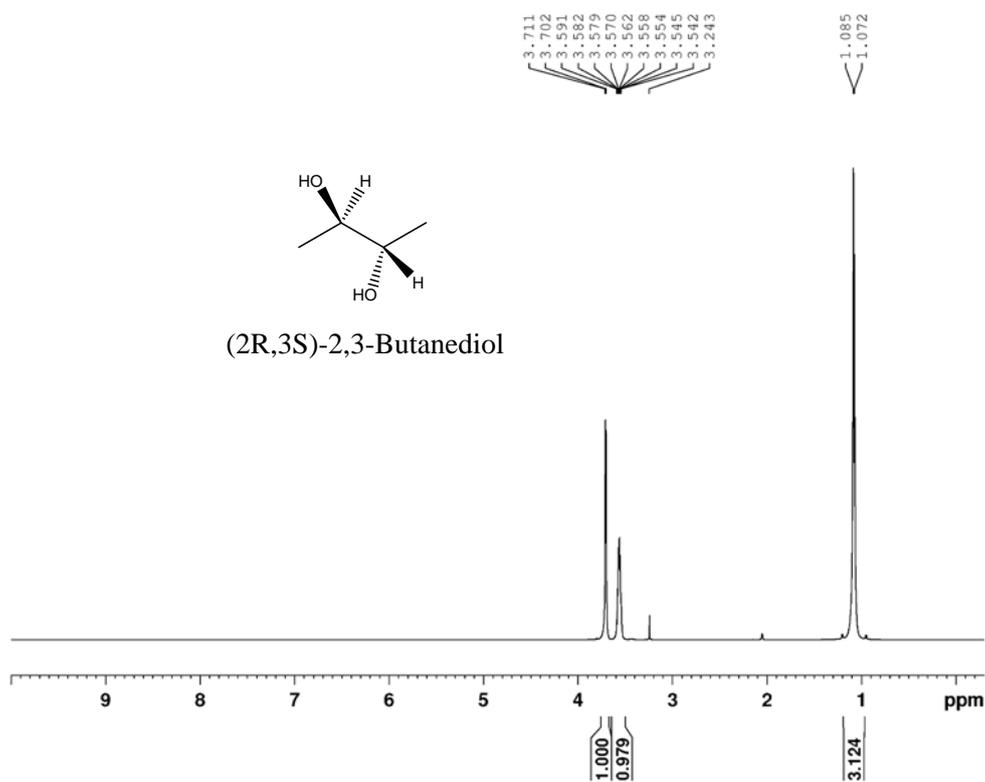


Fig. S2  $^1\text{H}$  NMR spectra of meso 2,3-butanediol.

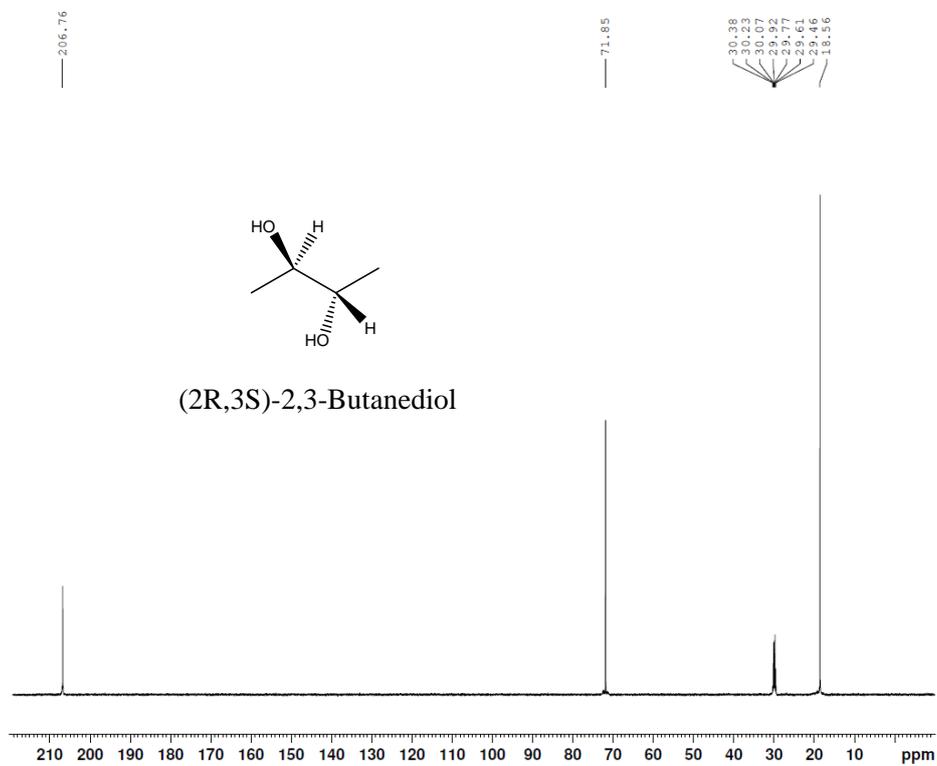


Fig. S3  $^{13}\text{C}$  NMR spectra of meso 2,3-butanediol.

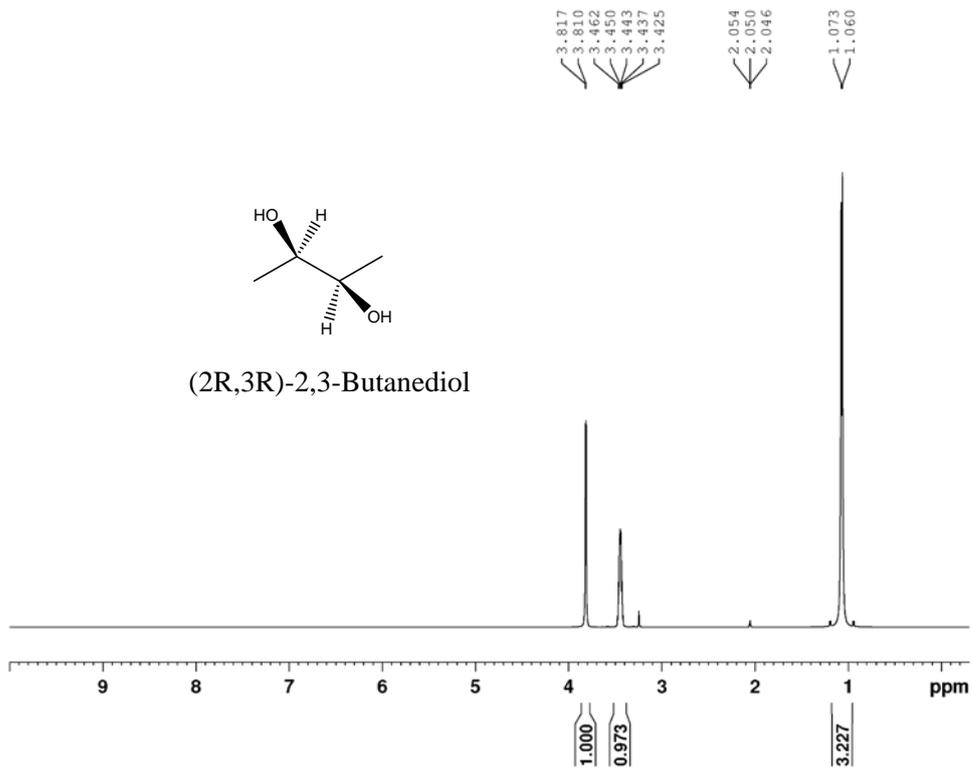


Fig. S4  $^1\text{H}$  NMR spectra of (2R,3R)-2,3-butanediol.

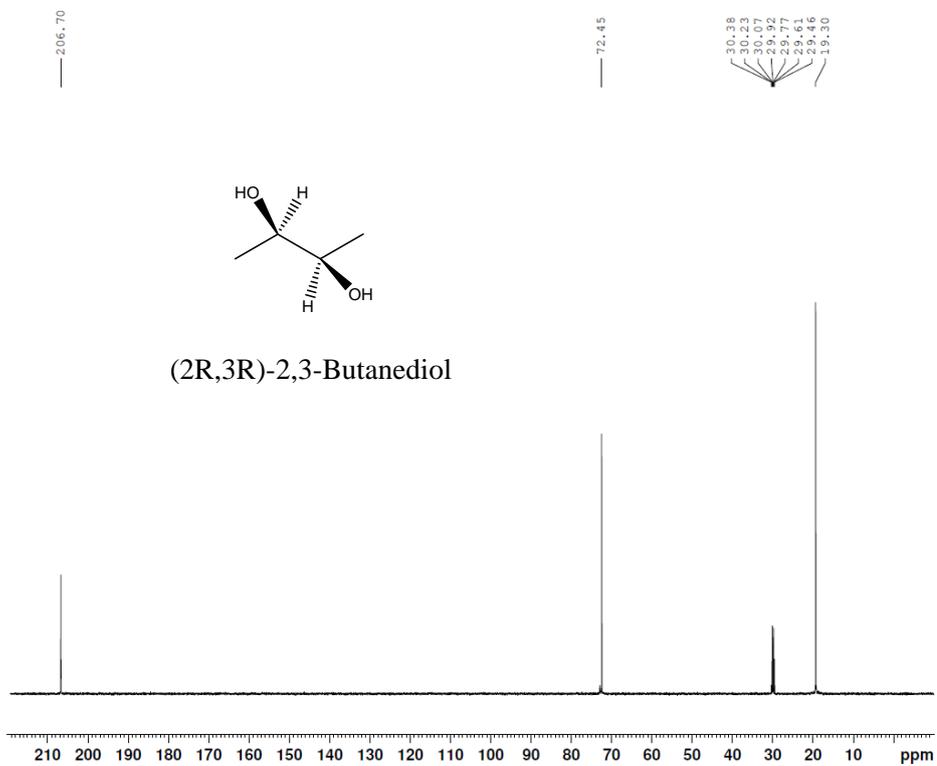
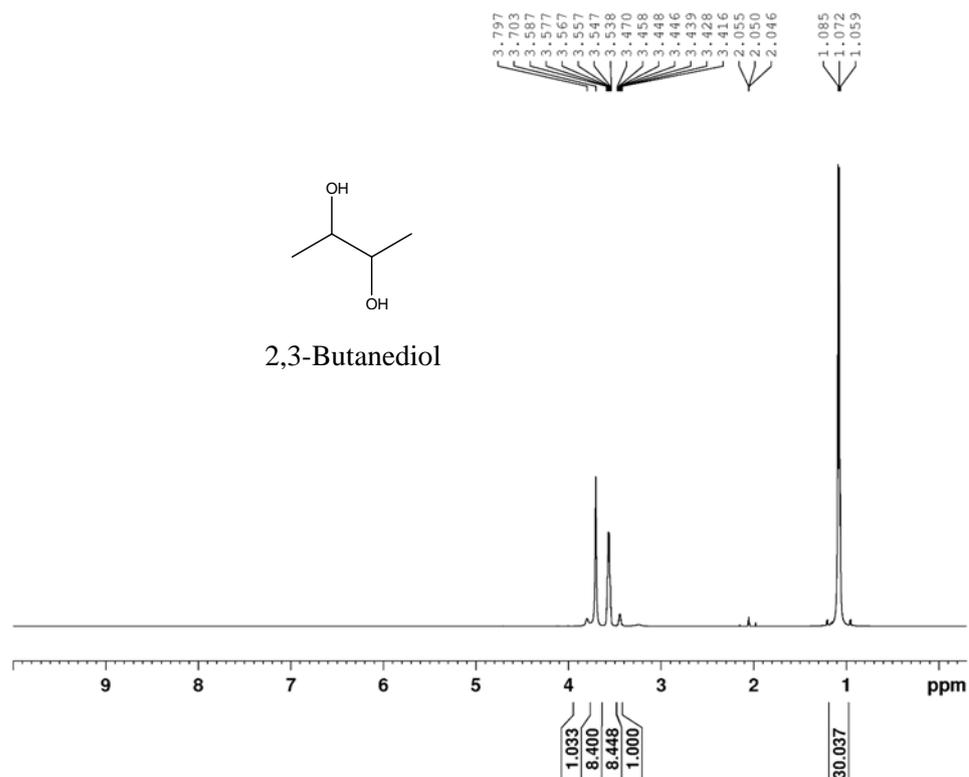
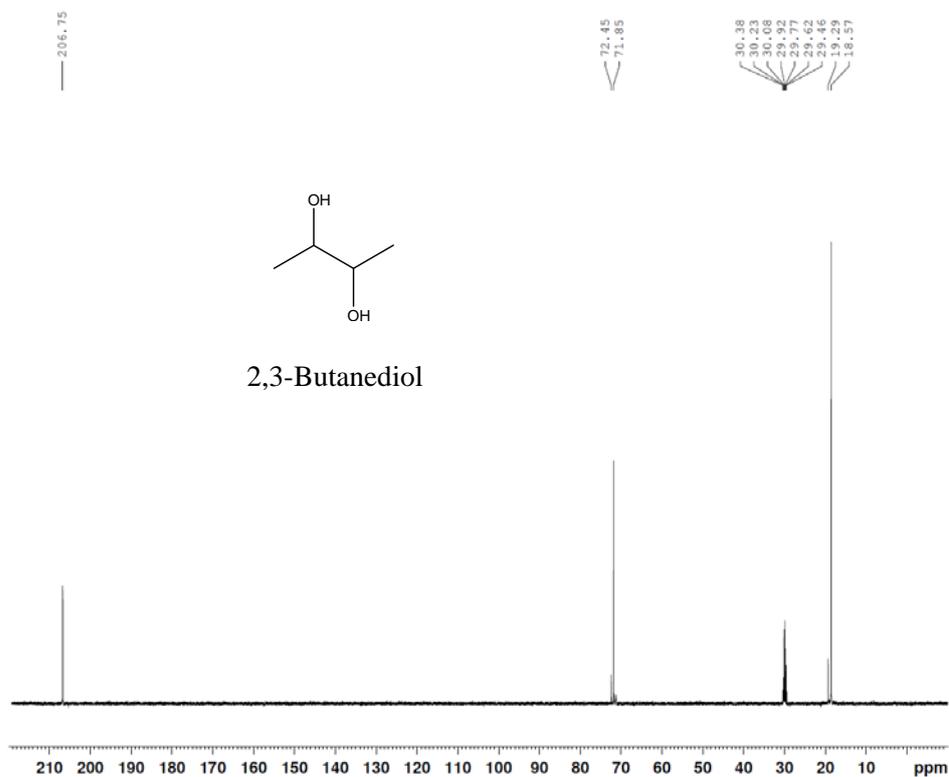


Fig. S5  $^{13}\text{C}$  NMR spectra of (2R,3R)-2,3-butanediol.

➤ NMR spectra of used 2,3-butenediol



**Fig. S6**  $^1\text{H}$  NMR spectra of used 2,3-butenediol (Menix international corporation, >97 % purity).



**Fig. S7**  $^{13}\text{C}$  NMR spectra of used 2,3-butenediol (Menix international corporation, >97 % purity).

➤ NMR spectra of esterification products

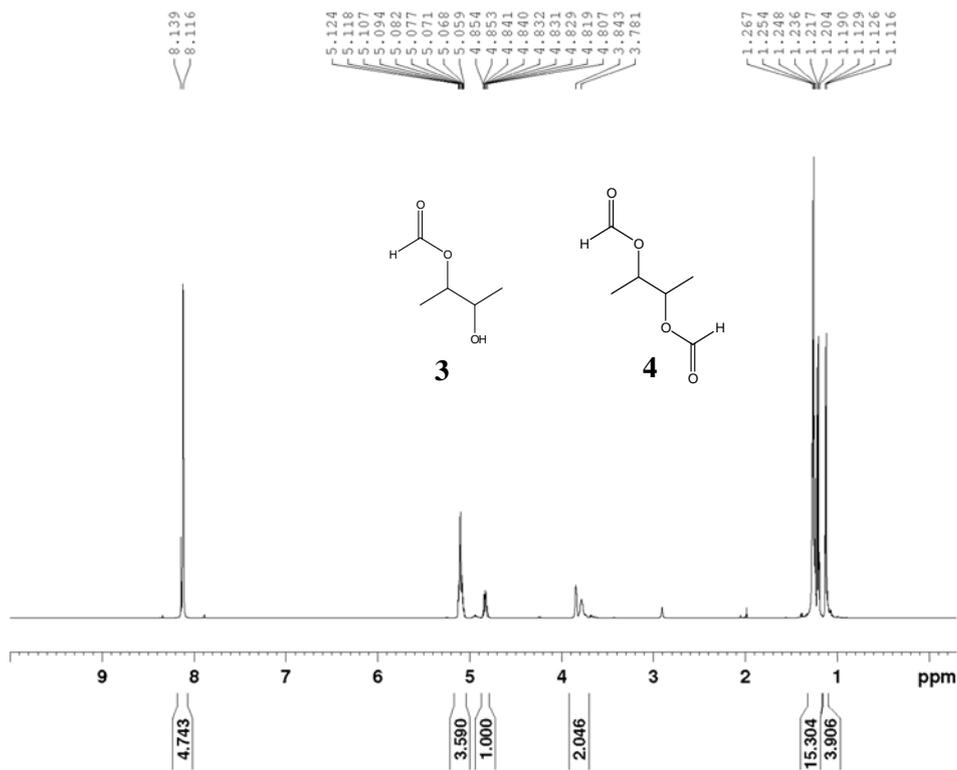


Fig. S8 <sup>1</sup>H NMR spectra of product 3 and 4.

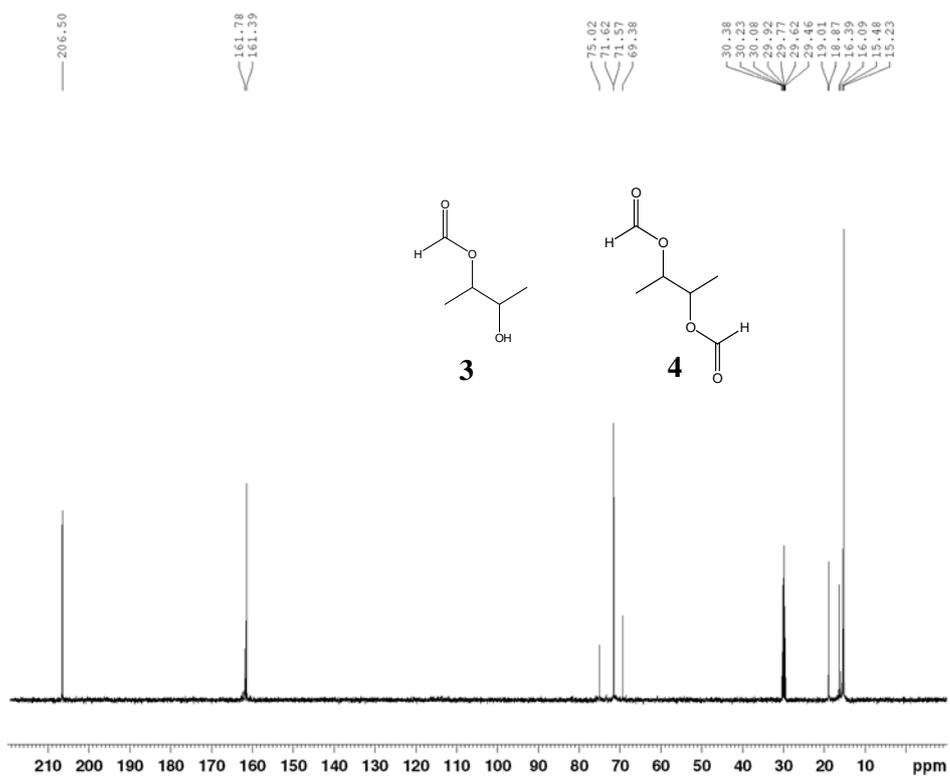
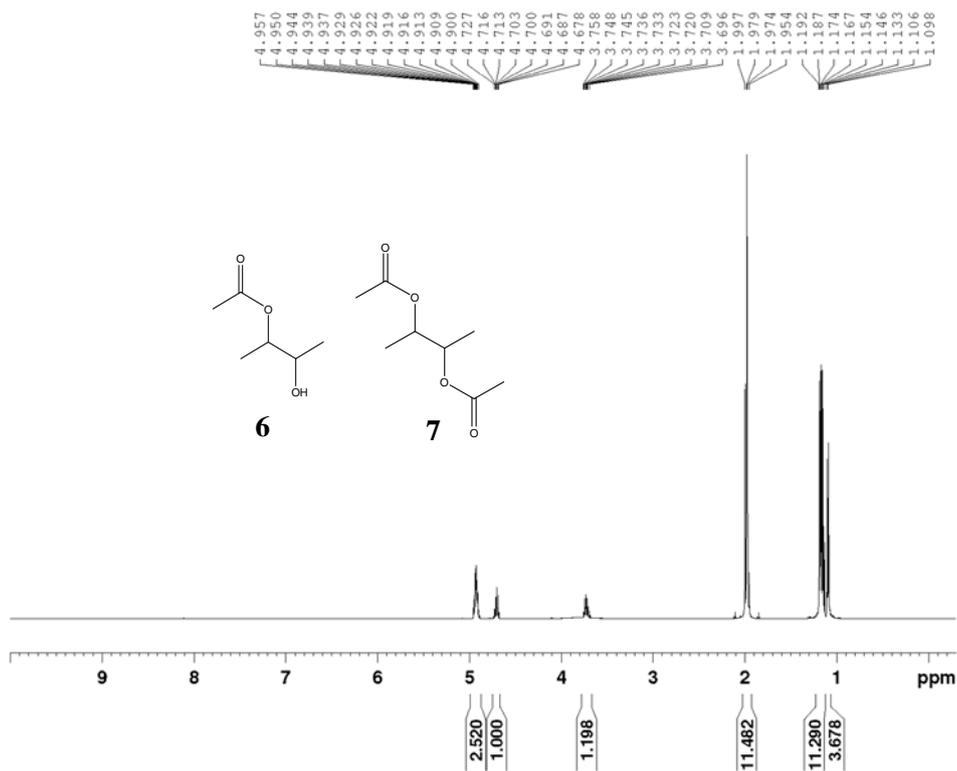
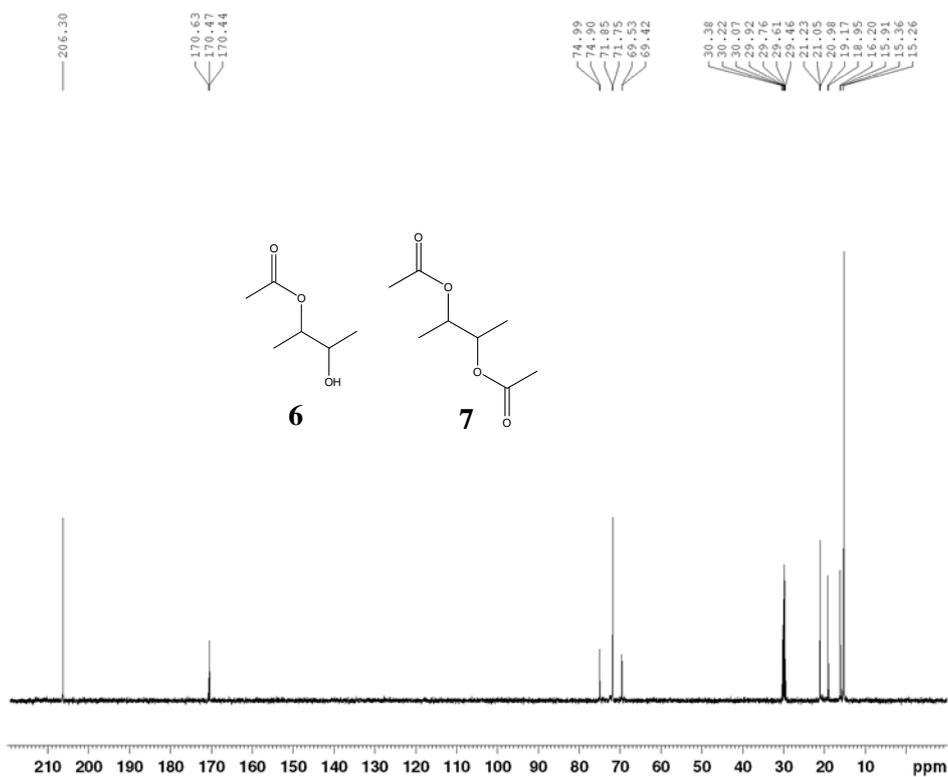


Fig. S9 <sup>13</sup>C NMR spectra of product 3 and 4.



**Fig. S10**  $^1\text{H}$  NMR spectra of product **6** and **7**.

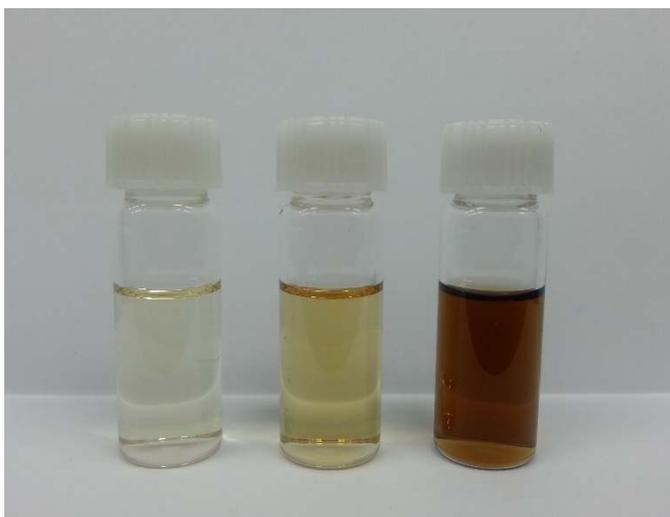


**Fig. S11**  $^{13}\text{C}$  NMR spectra of product **6** and **7**.

➤ **Photograph of esterification products**

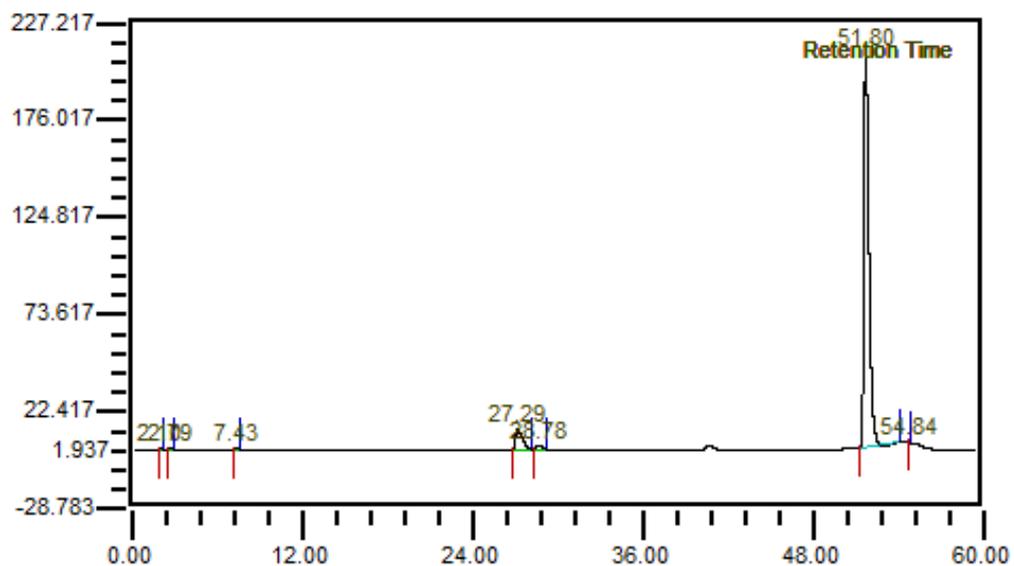


**Fig. S12** Photograph showing the color change of the esterification products (Fig. 1) as a function of time; 1 h (left), 3 h (middle), and 5 h (right).

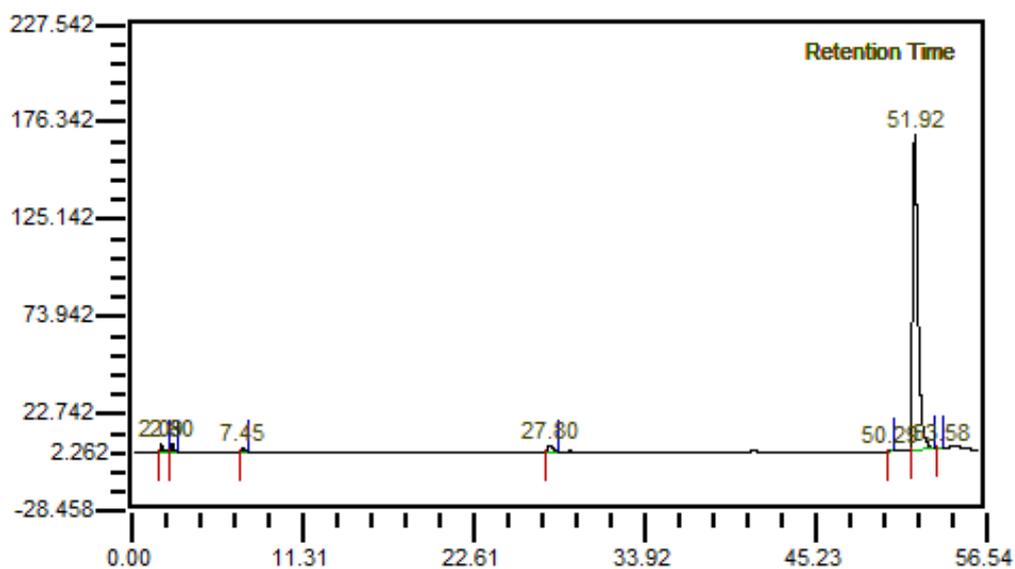


**Fig. S13** Photograph showing the color change of the esterification products (Fig. 2) as a function of time; 3 h (left), 7 h (middle), and 10 h (right).

➤ Gas phase stream



**Fig. S14** GC chromatogram of the gas phase obtained from the pyrolysis of product 4 (Figure 1, 500 °C, 5 h, > 93 % purity by GC).



**Fig. S15** GC chromatogram of the gas phase obtained from the pyrolysis of product 7 (Figure 1, 500 °C, 5 h, > 95 % purity by GC).

➤ NMR spectra of esterification product using model mixture

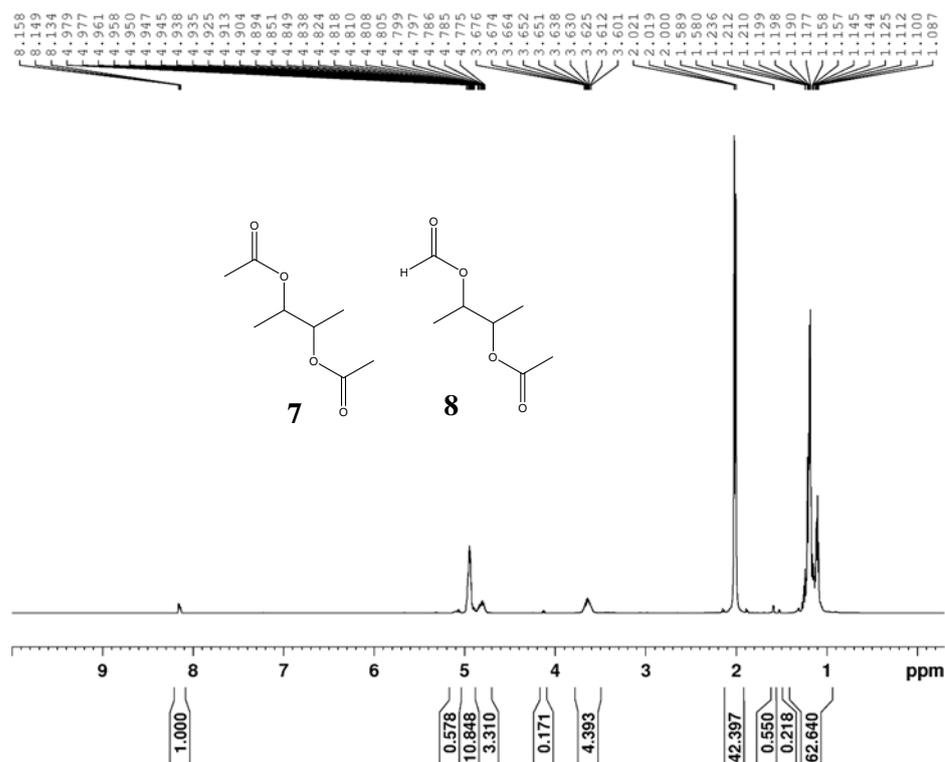


Fig. S16 <sup>1</sup>H NMR spectra of product 7 and 8.

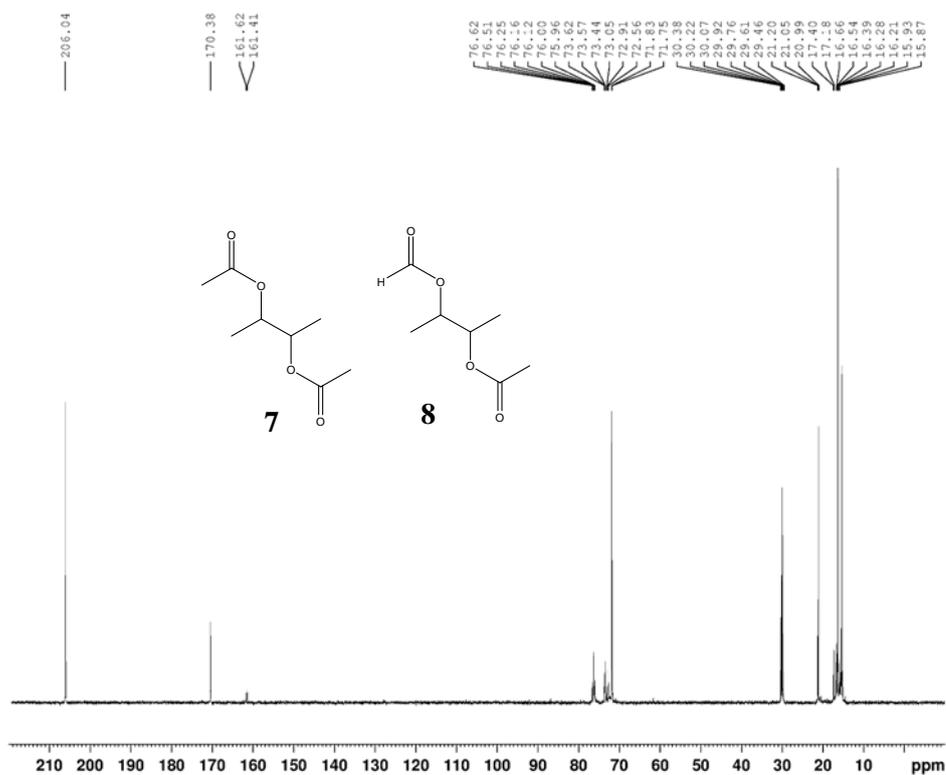


Fig. S17 <sup>13</sup>C NMR spectra of product 7 and 8.

## References

- 1S X. J. Ji, H, Huang, and P. K. Ouyang, *Biotechnol. Adv.*, 2011, **29**, 351.