

Supplementary Information

Development of an Analytical Method for Identification and Quantification of Glycerol Ethers

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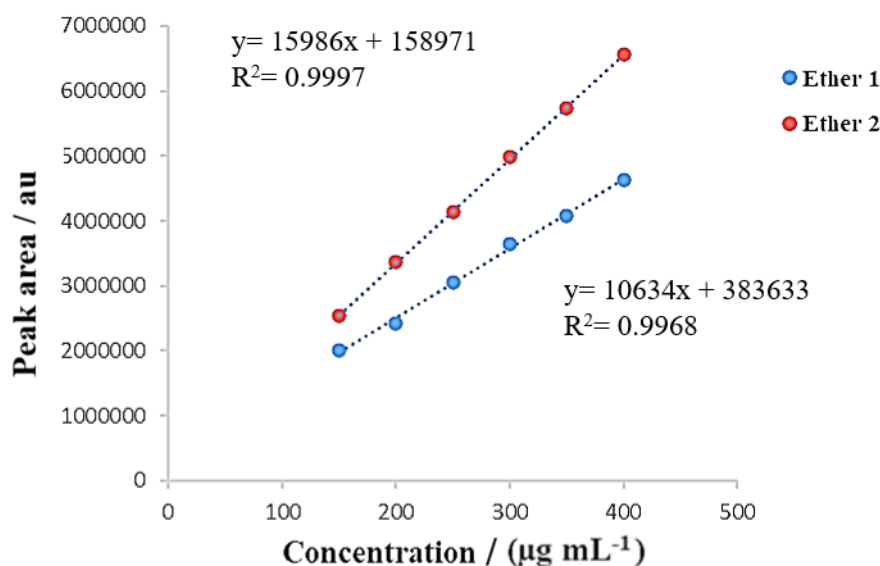


Figure S1. Analytical curves of ether 1 and ether 2 standards, in the concentration range of 150-400 µg L⁻¹.

Table S1. Analysis of variance (ANOVA) for analytical curve data of ether 1

Effect	Degrees of freedom	Squared sum	Squared mean	<i>F</i> -calculated	<i>F</i> -tabulated (95%)
Regression	1	3.282×10^{13}	3.282×10^{13}	66.130	0.004
Residue	10	4.963×10^{12}	4.963×10^{11}	—	—
Total	11	—	—	—	—

F: ratio of variance between groups; 95% confidence interval.

Table S2. Analysis of variance (ANOVA) for analytical curve data of ether 2

Effect	Degrees of freedom	Squared sum	Squared mean	<i>F</i> -calculated	<i>F</i> -tabulated (95%)
Regression	1	6.224×10^{13}	6.224×10^{13}	55.652	0.004
Residue	10	1.118×10^{13}	1.118×10^{12}	—	—
Total	11	—	—	—	—

F: ratio of variance between groups; 95% confidence interval.

Table S3. Results of the regression study of the curves for ether 1 and ether 2 using the Excel 2013 statistical program

	Ether 1	Ether 2
Correlation coefficient	0.9984	0.9998
SD _a	303.35	137.64
SD _b	87351	39633
<i>p</i> -value	0.012	0.016
<i>t</i> -test	4.39	4.11

SD: standard deviation; SD_a: standard deviation of intersection; SD_b: standard deviation of variable x.

Gas chromatography-mass spectrometry (GC-MS)

The reaction was also analyzed using a gas chromatograph-mass spectrometer (GC-MS, GCMS-QP2010 Plus, Shimadzu, Japan) equipped with an automatic injection sampler (AOC-20i, Shimadzu). The separation was performed on a silica capillary column (ZB-FFAP; nitroterephthalic acid-modified polyethylene glycol, with 30 m $\times$ 0.25 mm internal diameter (i.d.), 0.25 μ m film thickness). The sample was injected with a constant helium gas (5.0) flow rate of 1.63 mL min⁻¹. The injector temperature was set at 250 °C, and 1.0 μ L of sample was injected in split mode with a ratio of 50:1. Mass spectra were recorded over an m/z range of 35-500. The ion source temperature was maintained at 200 °C, and the interface temperature at 250 °C. The oven temperature program started at 90 °C (held for 3 min), increased to 230 °C at a rate of 20 °C min⁻¹ and held for 6 min, then raised to 250 °C at 10 °C min⁻¹ and held for 10 min. The total analysis time was 26.67 min.

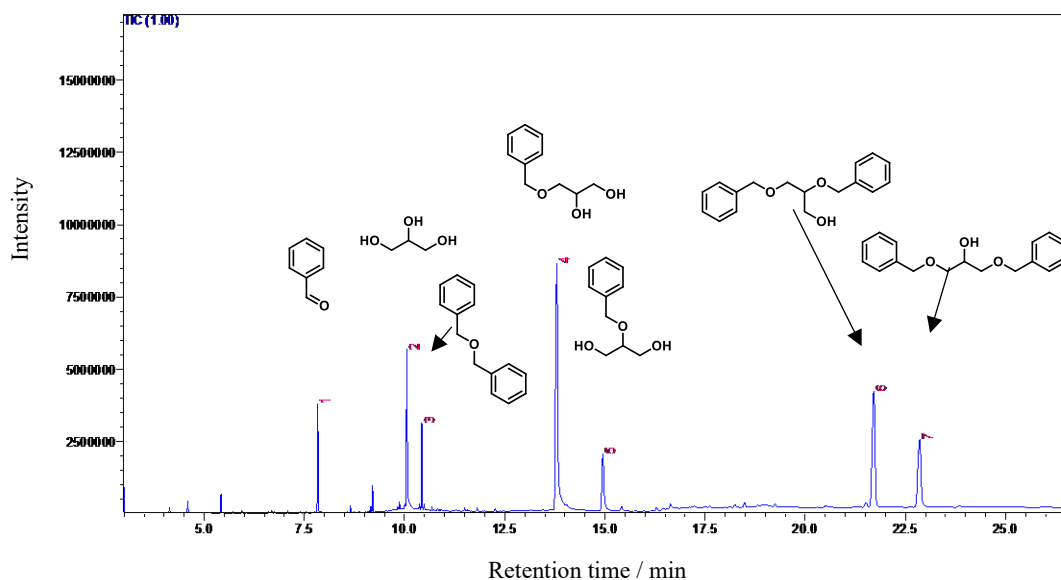


Figure S2. Chromatogram of reaction products from the etherification of glycerol with benzyl alcohol. **1**: benzyl alcohol; **2**: glycerol; **3**: benzyl ether; **4**: ether **1**; **5**: isomer-ether **1**; **6**: isomer-ether **2**; **7**: ether **2**, according to the NIST 08 equipment library.

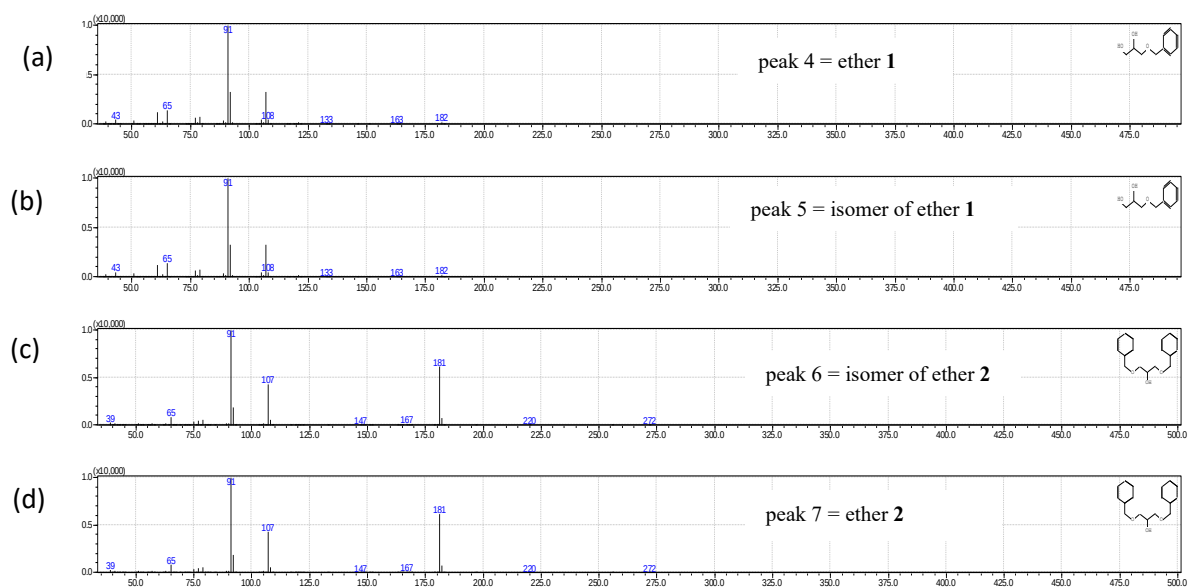


Figure S3. Mass spectra of (a) ether 1; (b) isomer of ether 1; (c) ether 2, and (d) isomer of ether 2.