Supplementary Information

Environmentally Friendly Process Design for Furan-based Long-chain Diesters Production Aiming for Bio-based Lubricant

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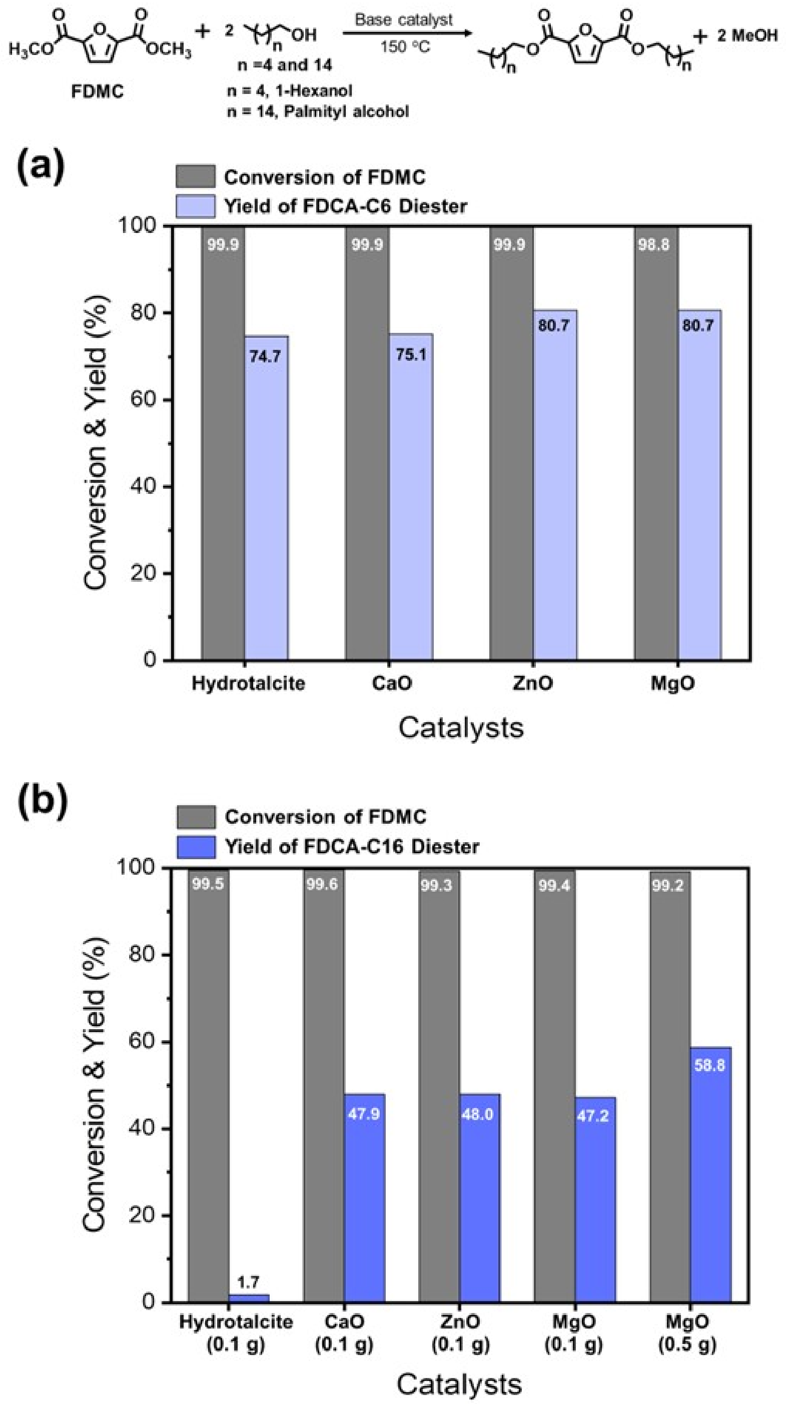

Figure S1. Transesterification of **FDMC** with (a) 1-hexanol (C6 alcohol) and (b) palmityl alcohol (C16 alcohol) over various base catalysts. Reaction conditions: FDMC (0.5 g, 2.7 mmol), alcohols (27 mmol), T = 150 °C, t = 20 h, catalyst amount (0.1 g), open reaction system.

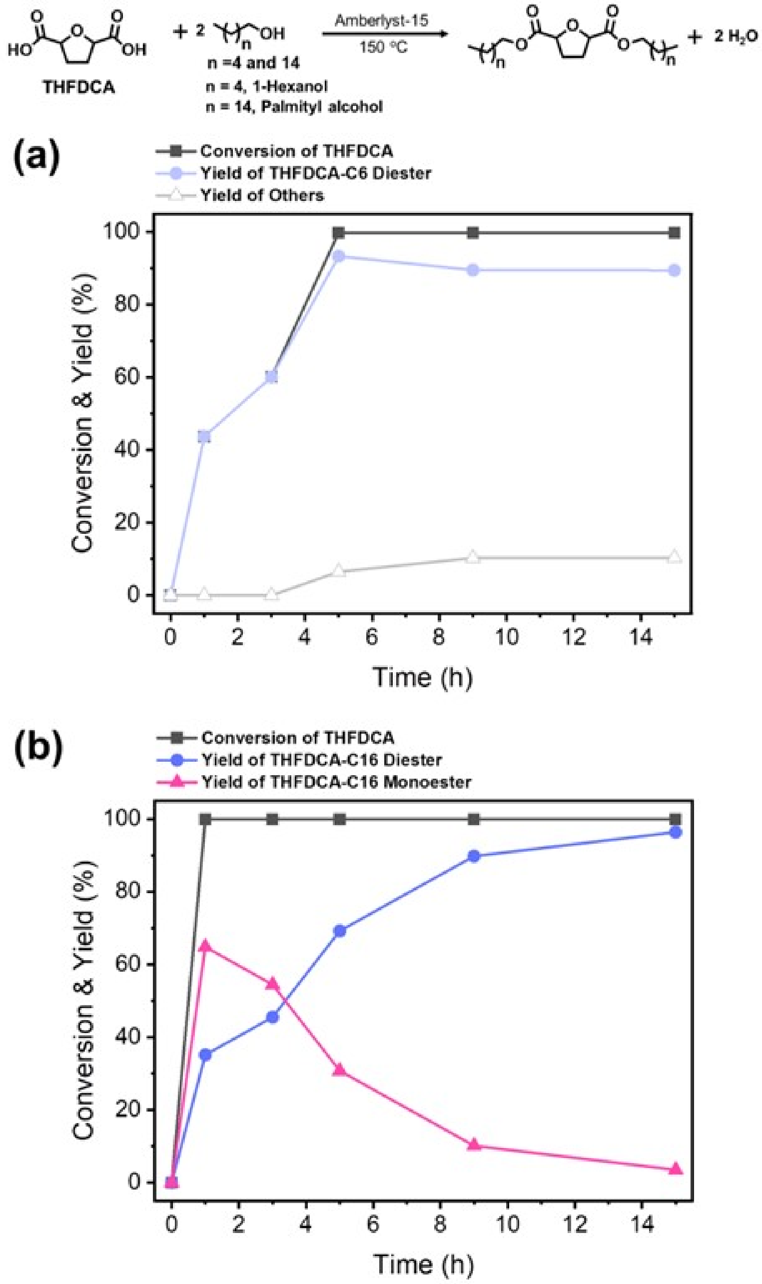

Figure S2. Effect of time in the esterification of **THFDCA** with (a) 1-hexanol (C6 alcohol) and (b) palmityl alcohol (C16 alcohol) over Amberlyst-15. Reaction conditions: THFDCA (0.5 g, 3.1 mmol), alcohols (31 mmol), Amberlyst-15 (0.1 g), cyclohexane (9 mL), T = 150 °C, with the Dean-Stark apparatus.

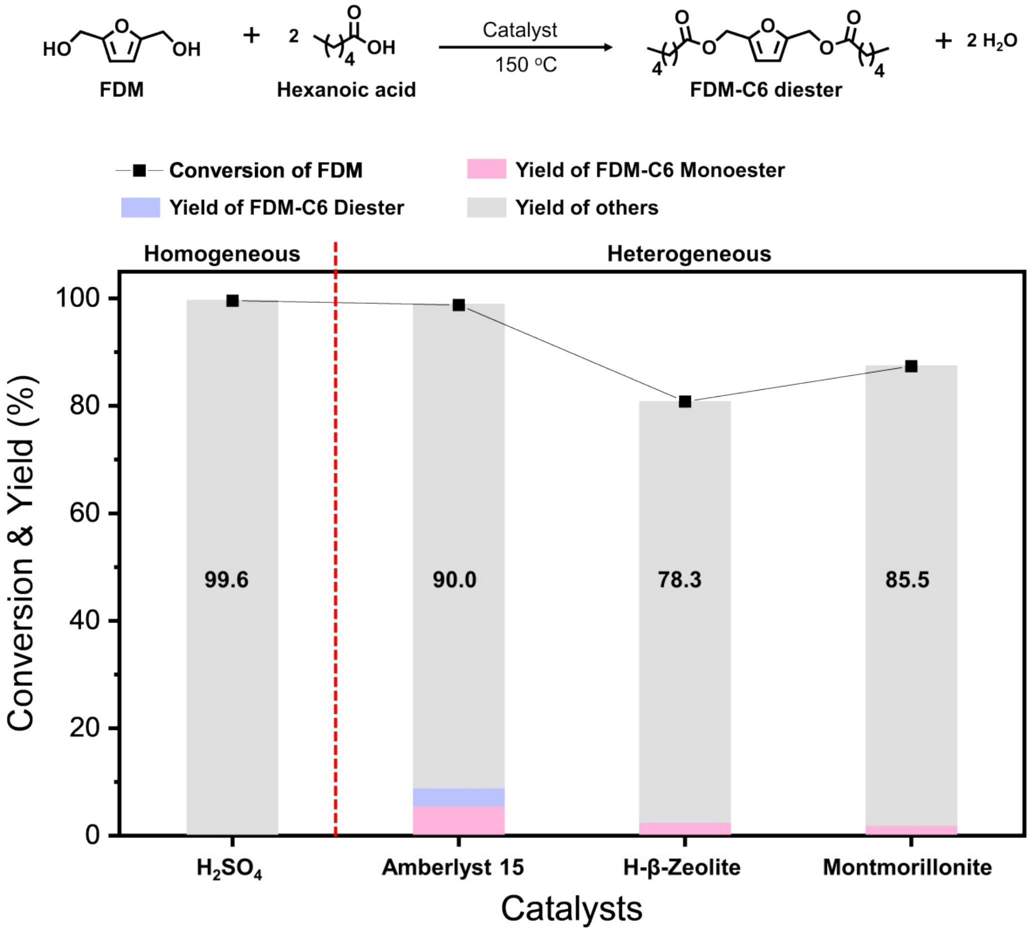

Figure S3. Esterification of **FDM** over various Brønsted catalysts. Reaction conditions: FDM (0.5 g, 3.9 mmol), hexanoic acid (39 mmol), Amberlyst-15 (0.1 g), cyclohexane (9 mL), T = 150 °C, t = 20 h, with the Dean-Stark apparatus.

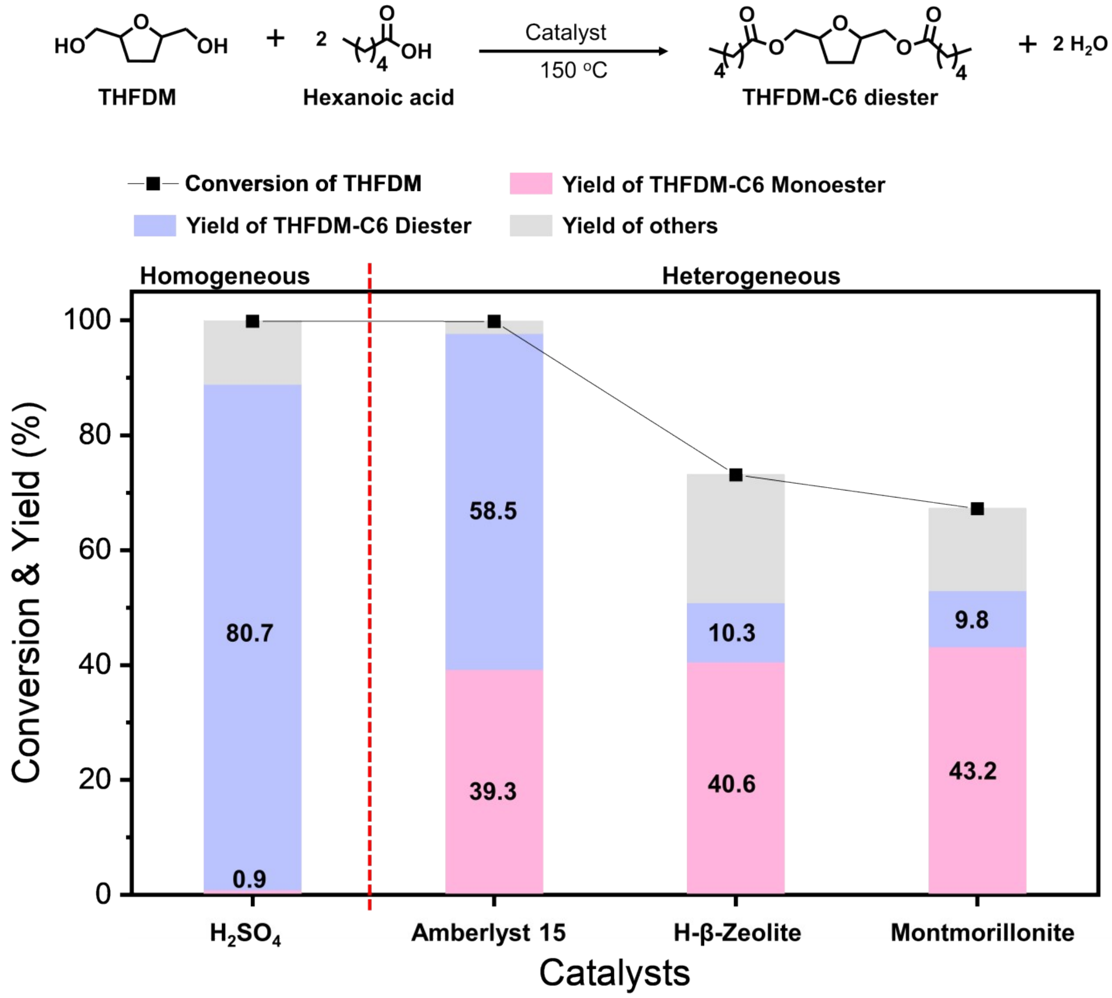

Figure S4. Esterification of **THFDM** with hexanoic acid (C6 fatty acid) over various acid catalysts. Reaction conditions: THFDM (0.5 g, 3.8 mmol), hexanoic acid (38 mmol), catalyst (0.1 g), cyclohexane (9 mL), T = 150 °C, t = 3 h, with the Dean-Stark apparatus.

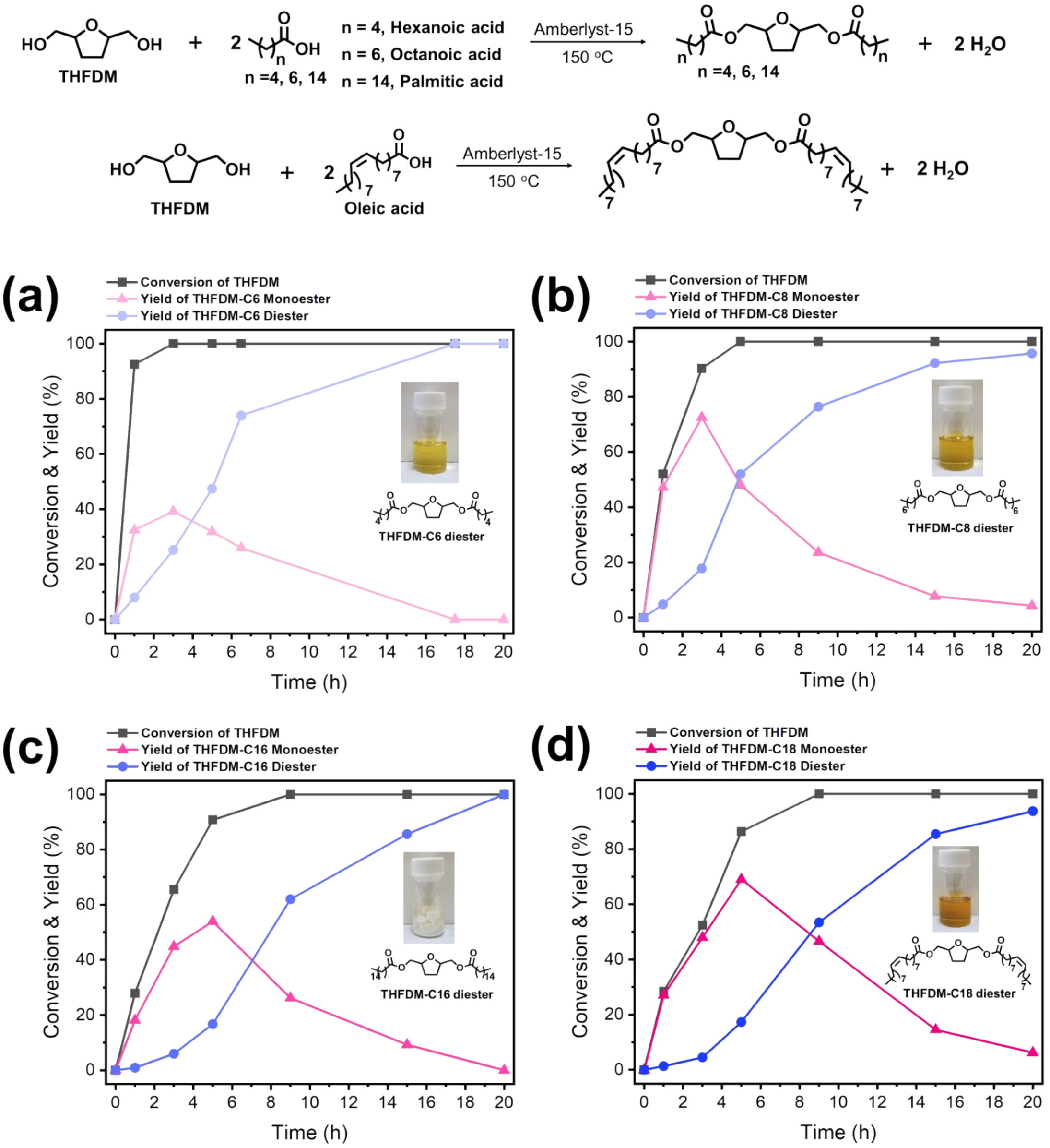

Figure S5. Effect of time in the esterification of **THFDM** with (a) hexanoic acid (C6 fatty acid), (b) octanoic acid (C8 fatty acid), (c) palmitic acid (C16 fatty acid), and (d) oleic acid (C18 fatty acid) over Amberlyst-15. Reaction conditions: THFDM (0.5 g, 3.8 mmol), fatty acids (38 mmol), Amberlyst 15 (0.1 g), cyclohexane (9 mL), T = 150 °C, with the Dean-Stark apparatus.

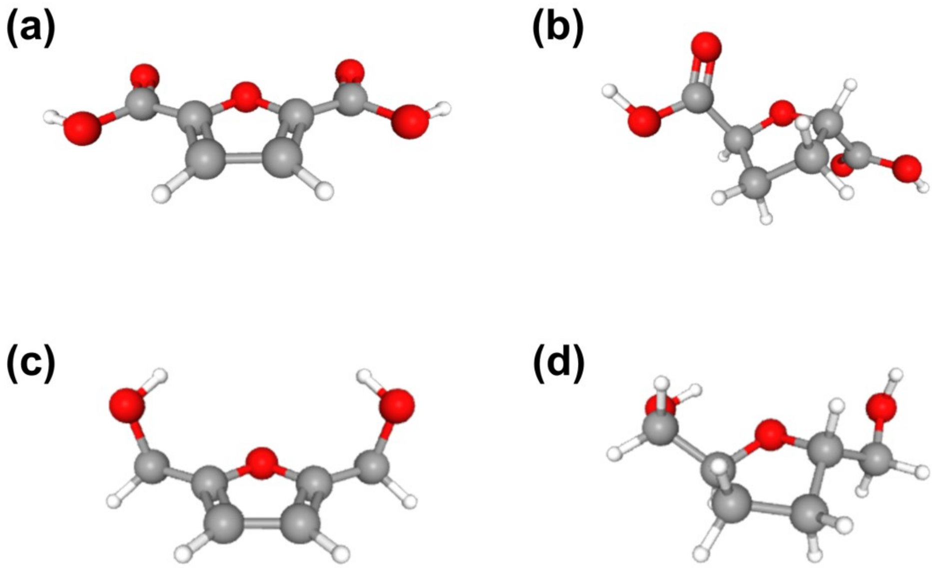

Figure S6. Molecular structure of furan compounds; (a) FDCA (b) THFDCA (c) FDM (d) THFDM

FDM and FDCA have double bonds in the furan ring, which means that the carbon atoms in the furan ring are planar structures due to their aromaticity. On the other hand, the carbon atoms in THFDM and THFDCA are single-bonded structures, causing distortion in the furan ring. S. P. Rao et al. reported that chemicals' melting points are related to molecular symmetry and size.[1] Based on this fact, the structural differences between furan and tetrahydrofuran affect melting points of furan compounds: FDCA (342 ^{o}C) > THFDCA (195–200 ^{o}C) > FDM (74–77 ^{o}C) > THFDM (-108.4 ^{o}C).

Large-scale synthesis of furan diesters

1. Synthesis of FDCA diesters

In a typical procedure for the transesterification of FDMC with fatty alcohols, FDMC (126 g, 0.68 mol) and ZnO (25.2 g) were placed in a round-bottomed flask, and fatty alcohols (2.74 mol, 4 equiv. to FDMC) were added. The reactions were carried out in an open vessel system in the air atmosphere at 150 °C for 60 h.

For FDCA-C6 and FDCA-C8 diesters, the catalyst was removed by filtration after reaction. The final products were obtained by vacuum distillation to remove excess alcohols.

For FDCA-C16 diester, the catalyst was quickly removed by filtration before solidification. The FDCA-C16 diester was then separated by recrystallization in acetone.

For FDCA-C18 diester, the catalyst was removed by filtration after reaction. Methanol was added to the crude product, causing phase separation between the oleyl alcohol-methanol solution and the FDCA-C18 diester. To obtain pure FDCA-C18 diester, flash column chromatography using hexane/ethyl acetate (15/1) as eluent was conducted. The final product was obtained by evaporating the eluent.

2. Synthesis of THFDCA diesters

In a typical procedure for the esterification of THFDCA with fatty alcohols, THFDCA (110 g, 0.69 mol) and Amberlyst-15 (5 g) were placed in a round-bottomed flask, and fatty alcohols (2.75 mol, 4 equiv. to THFDCA) were added. Cyclohexane (100 ml) was then added to the reaction mixture as a reflux solvent. The Dean-Stark with a condenser was installed on top of the flask, and the esterifications were carried out at 150 °C for 48 h.

For THFDCA-C6 and THFDCA-C8 diesters, the catalyst was removed by filtration after reaction. The final products were obtained by vacuum distillation to remove excess alcohols.

For THFDCA-C16 diester, the catalyst was quickly removed by filtration before solidification. The THFDCA-C16 diester was then separated by recrystallization in acetone.

For THFDCA-C18 diester, the catalyst was removed by filtration after reaction. To obtain pure THFDCA-C18 diester, flash column chromatography using hexane/ethyl acetate (4/1) as eluent was conducted. The final product was obtained by evaporating the eluent.

3. Synthesis of FDM diesters

Acyl chlorides (fatty acid chlorides) were used for the large-scale synthesis of FDM diesters. In a typical procedure, FDM (30 g, 0.23 mol) was added to dry CH_2Cl_2 (700 mL). Triethylamine (69 mL, 4 equiv. to FDM), N,N'-dimethylaminopyridine (0.98 g), and fatty acid chlorides (0.7 mol, 3 equiv. to FDM) were then added dropwise to prevent explosive reactions. After the substrates were completely converted to diesters at room temperature over 15 h, unreacted fatty acid chlorides were hydrolyzed to fatty acids by addition of water.

For FDM-C6, FDM-C8, and FDM-C18 diesters, the separated organic layer was washed with 2 M Na_2CO_3 solution to eliminate fatty acids which were transformed into their sodium salts. After washing the products with D.I. water 3 times, the final products were obtained after evaporating CH_2Cl_2.

For FDM-C16 diester, all solvents in crude product were removed by vacuum evaporation. Water (600 mL) and hexane (600 mL) were then added to the resulting solution. The organic layer was separated using a separatory funnel, and the hexane was removed by evaporation. The FDM–C16 diester was finally purified by recrystallization in ethanol.

4. Synthesis of THFDM diesters

In a typical procedure for the esterification of THFDM with fatty acids, THFDM (110 g, 0.83 mol) and Amberlyst-15 (5 g) were placed in a round-bottomed flask, and fatty acids (2.49 mol, 3 equiv. to THFDM) were added. Cyclohexane (100 ml) was then added to the reaction mixture as a reflux solvent. The Dean-Stark with condenser was installed on top of the flask, and the esterifications were carried out at 150 ℃ for 48 h.

For THFDM-C6, THFDM-C8, and THFDM-C18 diesters, after removing the catalyst by filtration, ethyl acetate (500 mL) was added to the mixture to extract organic components. The fatty acids were removed by transforming it into its sodium salts by washing with 2 M Na_2CO_3 solution. After washing the products with D.I. water 3 times, the final products were obtained after evaporating ethyl acetate.

For THFDM-C16 diester, the catalyst was quickly removed by filtration before solidification. The THFDM-C16 diester was purified by recrystallization in ethanol.

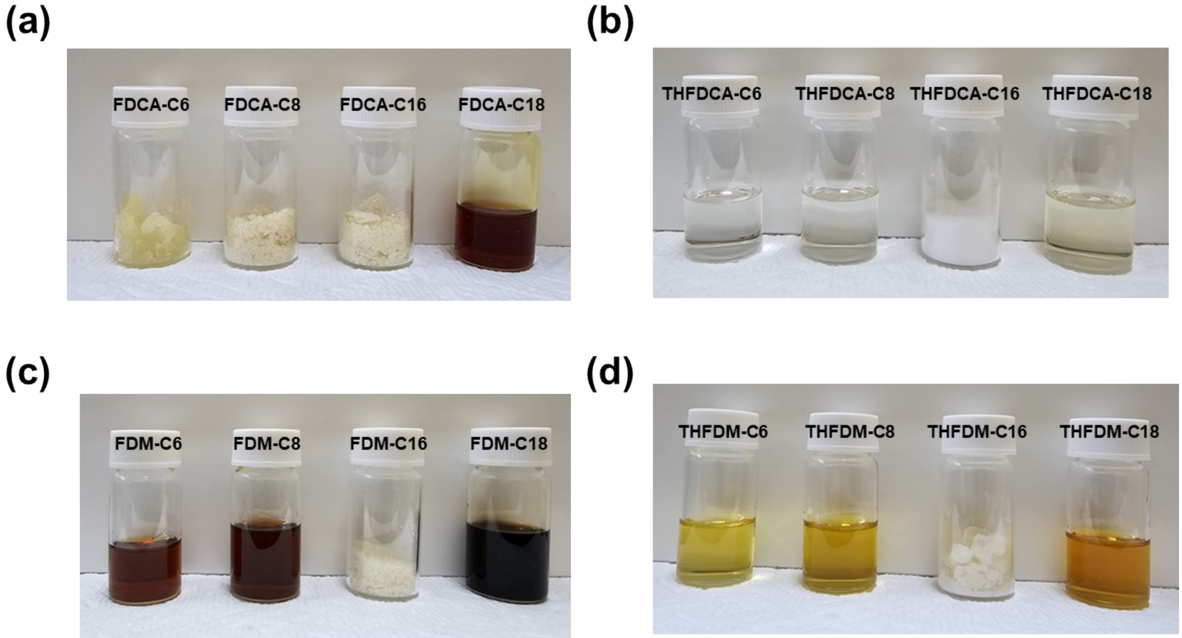

Figure S7. Pictures of synthesized furan diesters: (a) FDCA-based diesters, (b) THFDCA-based diesters, (c) FDM-based diesters, and (d) THFDM-based diesters.

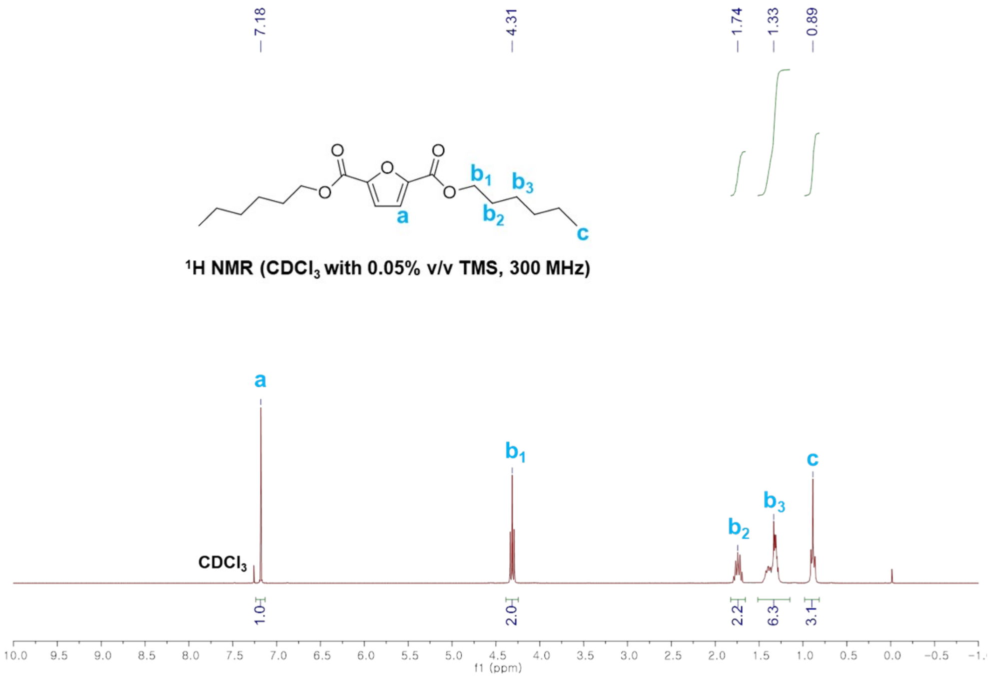

Figure S8. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDCA-C6** diester.

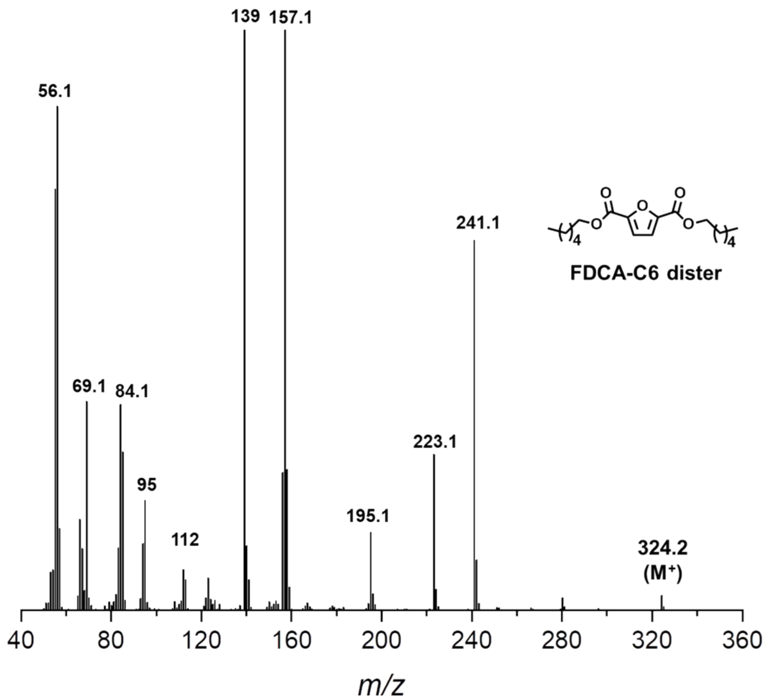

Figure S9. GC-MS total ion chromatogram (TIC) of purified **FDCA-C6** diester.

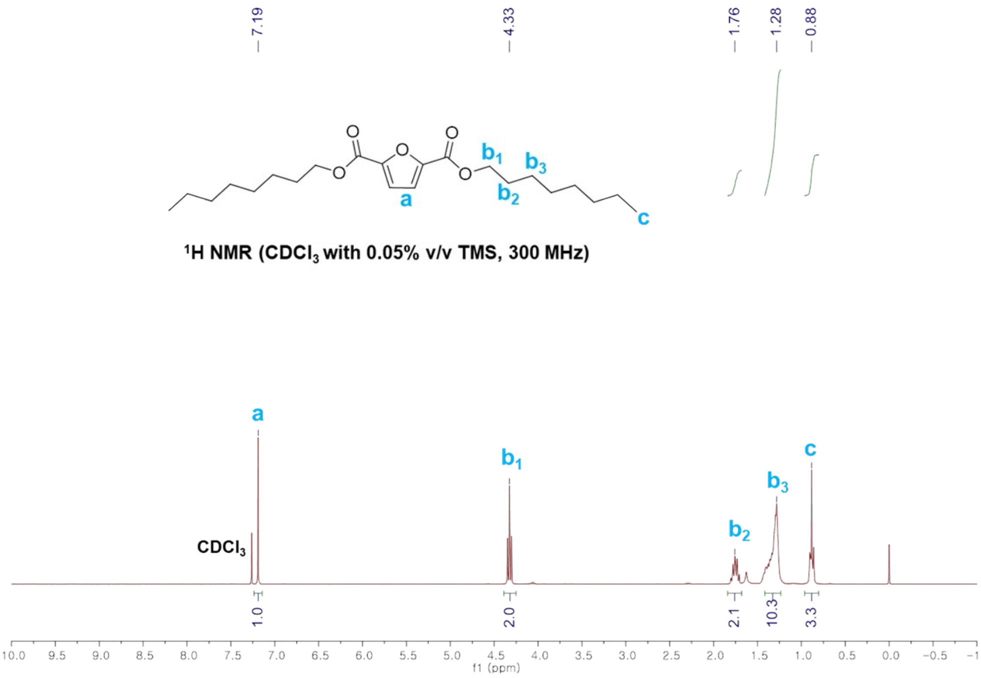

Figure S10. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDCA-C8** diester.

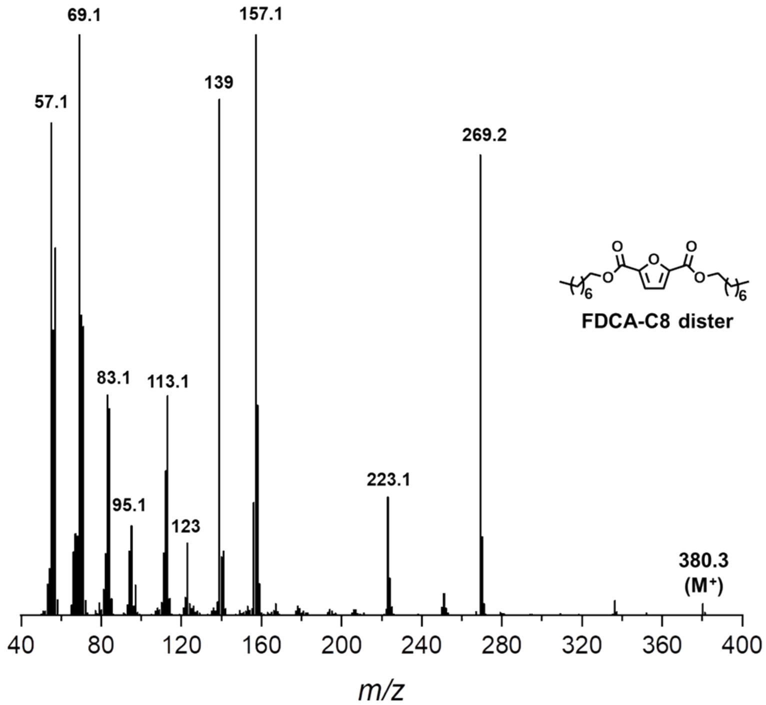

Figure S11. GC-MS total ion chromatogram (TIC) of purified **FDCA-C8** diester.

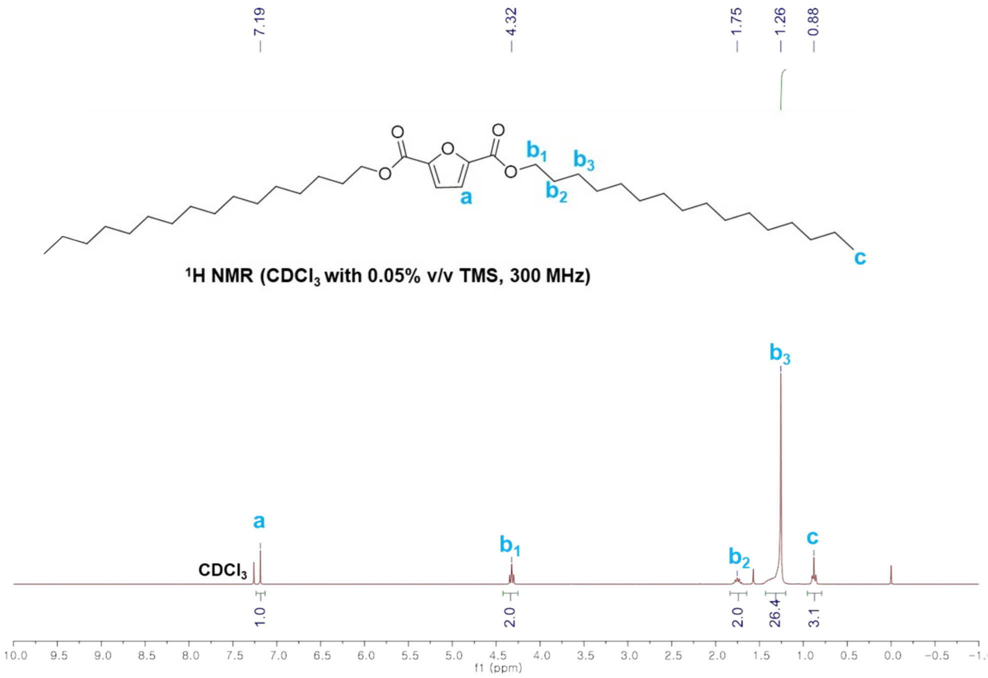

Figure 12. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDCA-C16** diester.

Figure S13. GC-MS total ion chromatogram (TIC) of purified **FDCA-C16** diester.

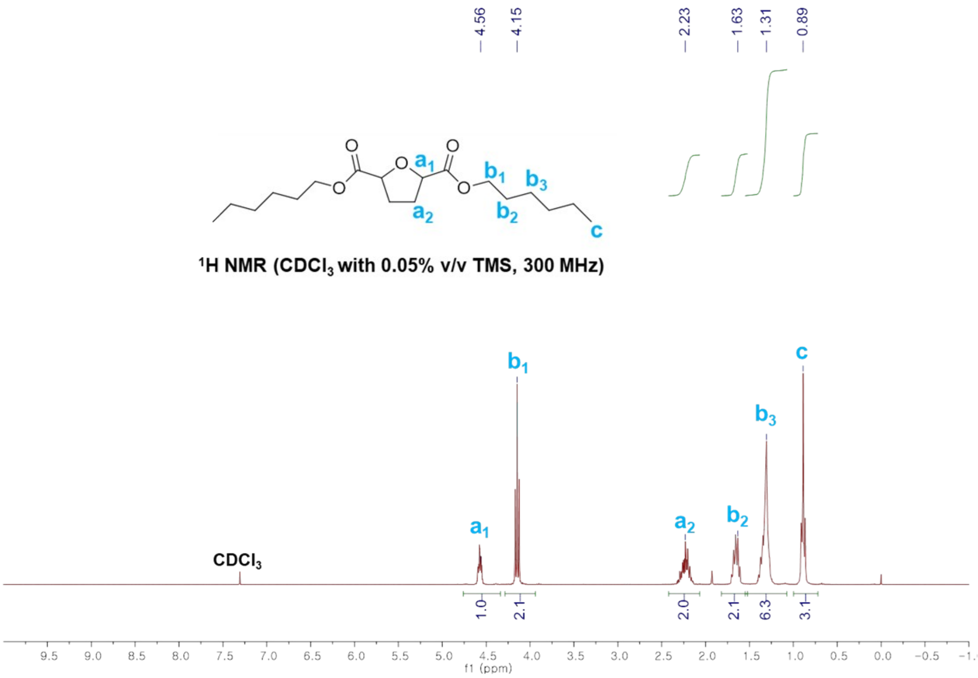

Figure S14. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDCA-C6** diester.

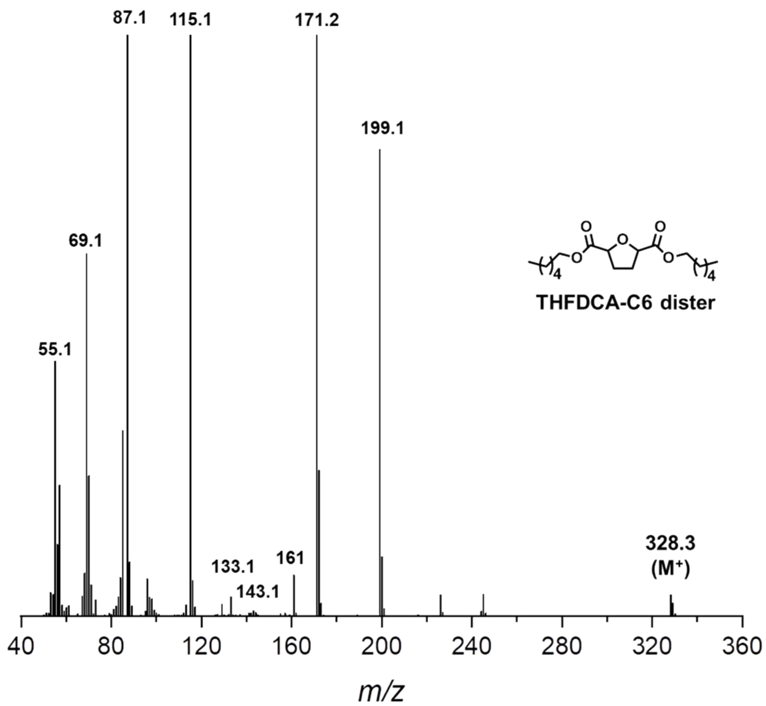

Figure S15. GC-MS total ion chromatogram (TIC) of purified **THFDCA-C6** diester.

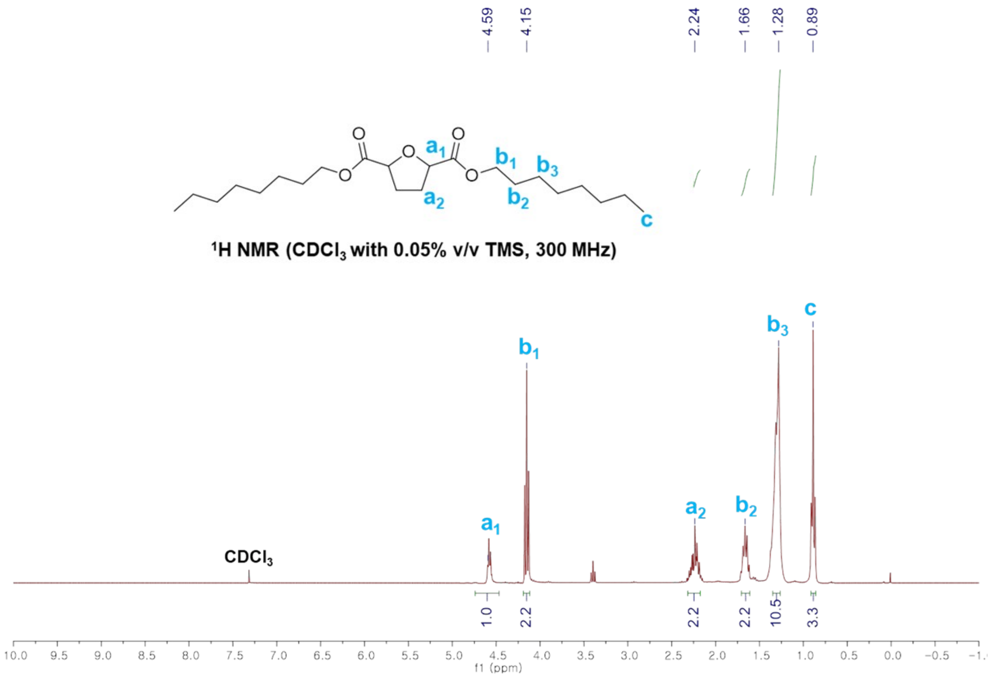

Figure S16. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDCA-C8** diester.

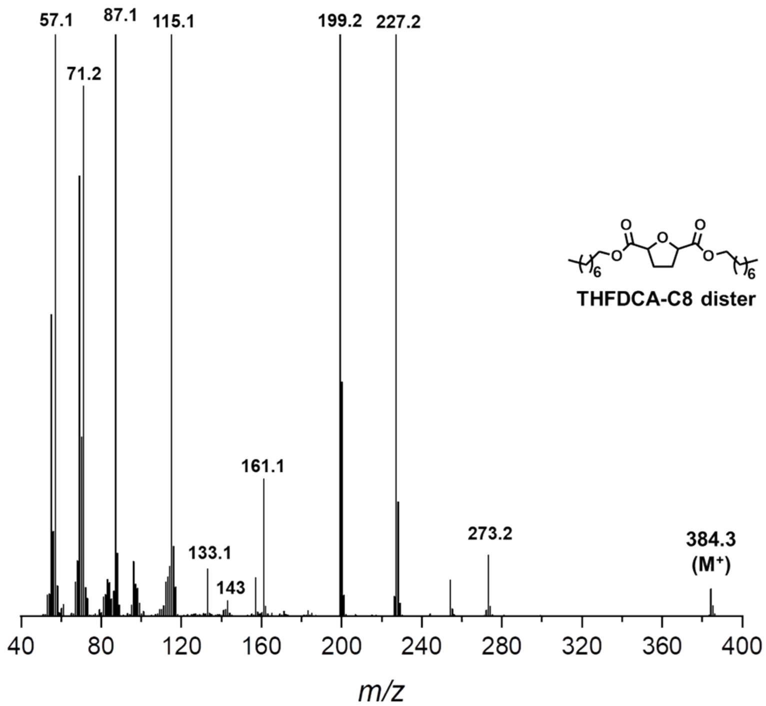

Figure S17. GC-MS total ion chromatogram (TIC) of purified **THFDCA-C8** diester.

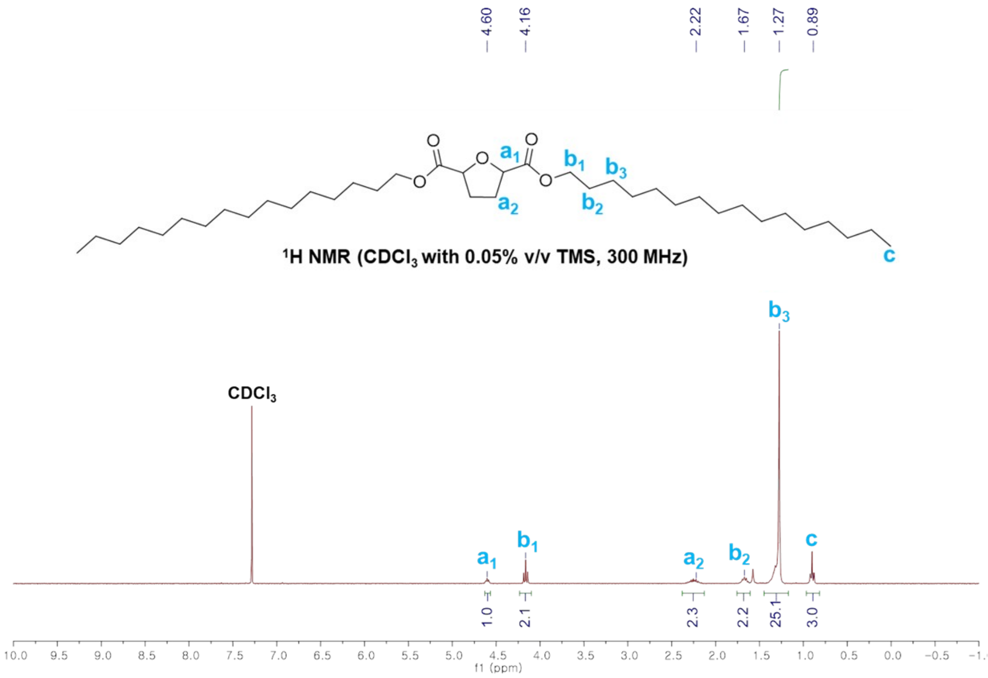

Figure S18. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDCA-C16** diester.

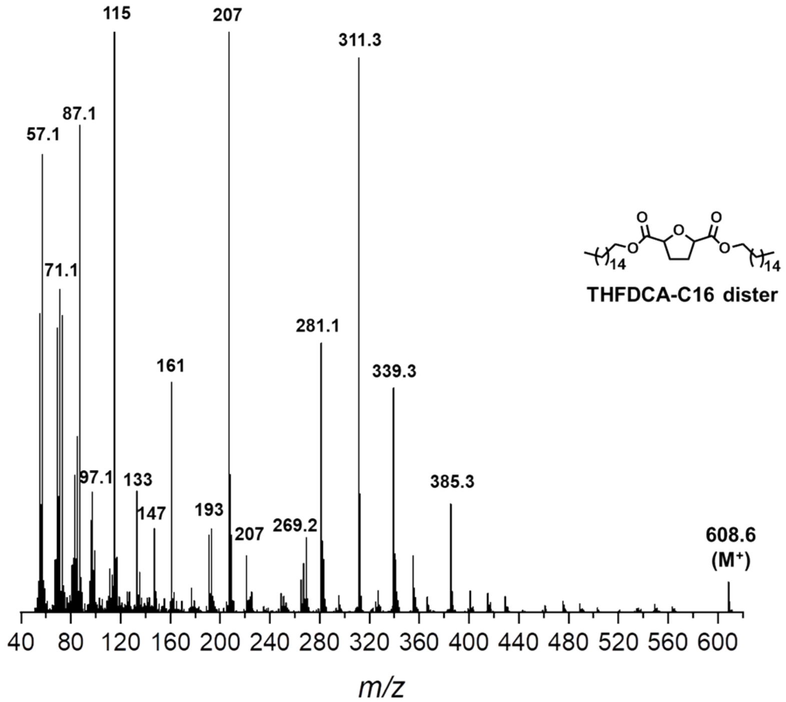

Figure S19. GC-MS total ion chromatogram (TIC) of purified **THFDCA-C16** diester.

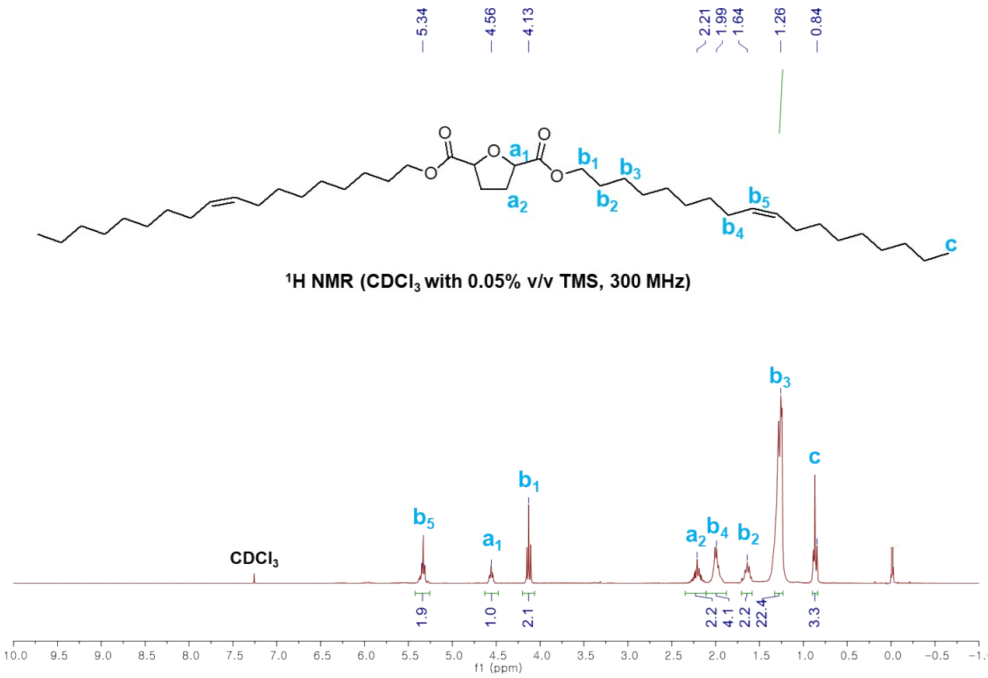

Figure S20. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDCA-C18** diester.

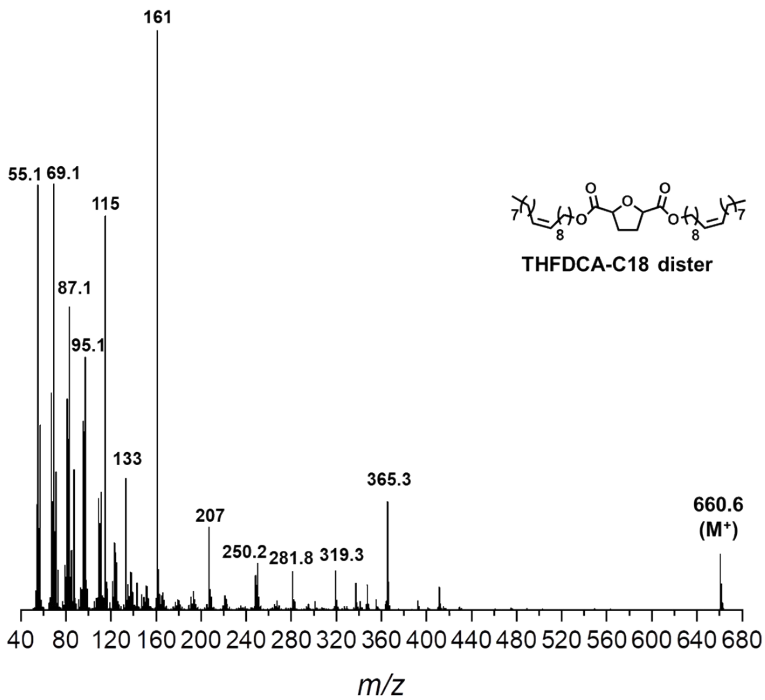

Figure S21. GC-MS total ion chromatogram (TIC) of purified **THFDCA-C18** diester.

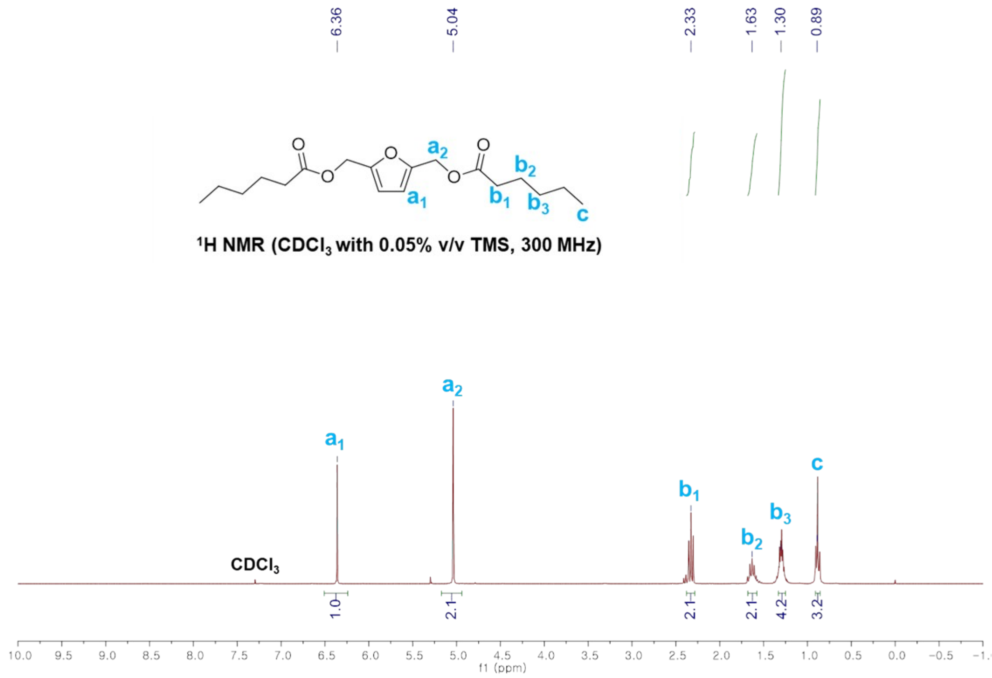

Figure S22. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDM-C6** diester.

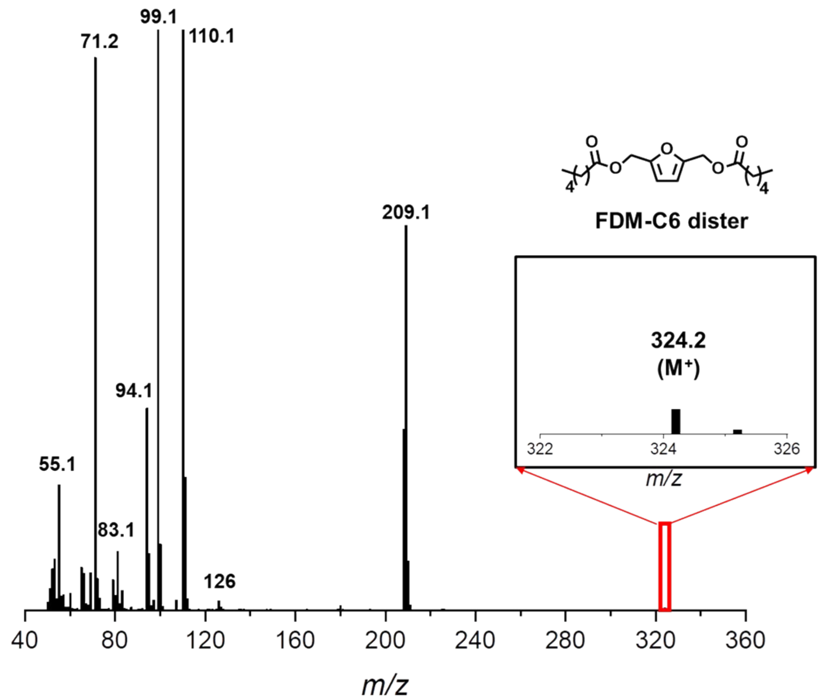

Figure S23. GC-MS total ion chromatogram (TIC) of purified **FDM-C6** diester.

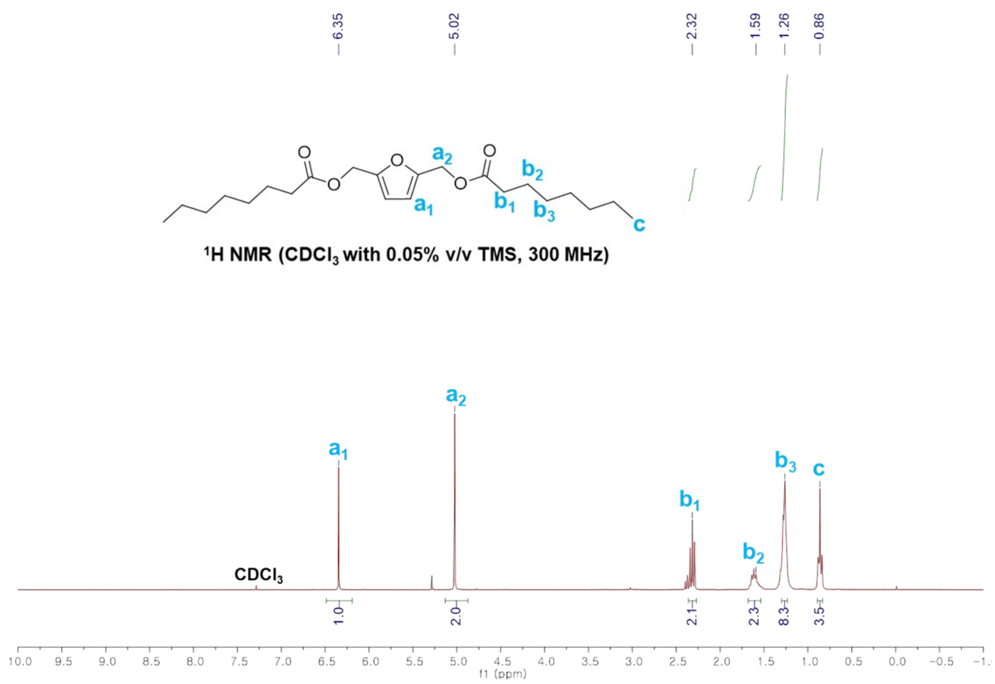

Figure S24. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDM-C8** diester.

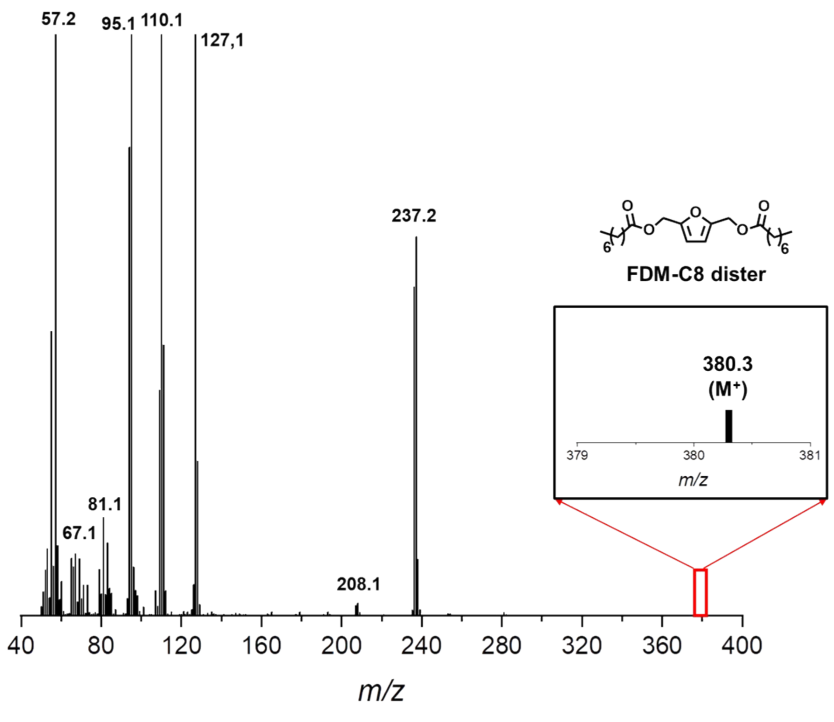

Figure S25. GC-MS total ion chromatogram (TIC) of purified **FDM-C8** diester.

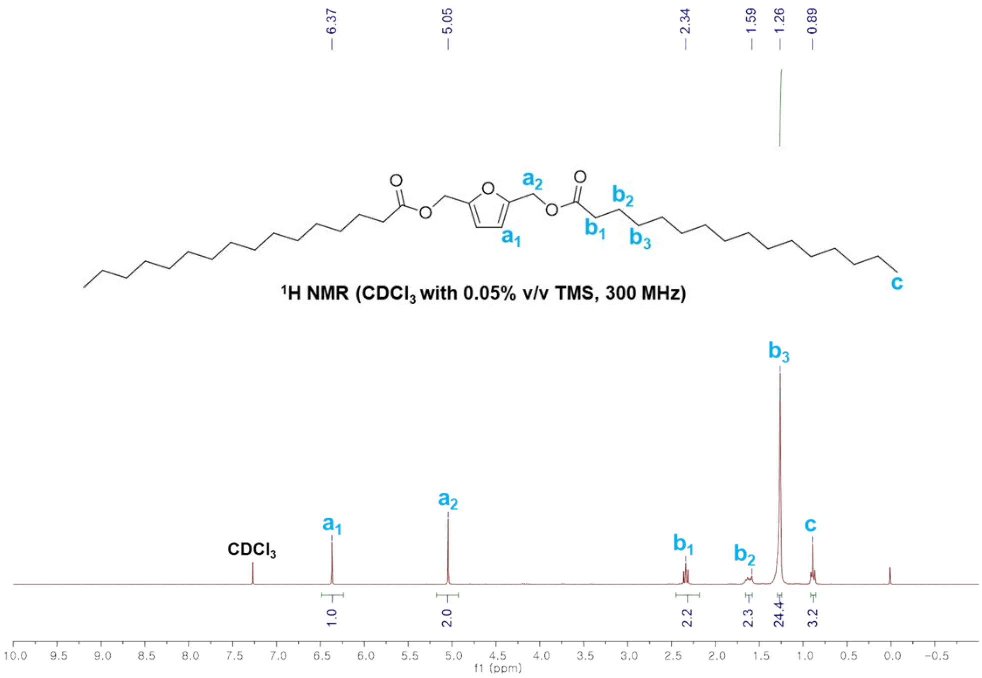

Figure S26. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDM-C16** diester.

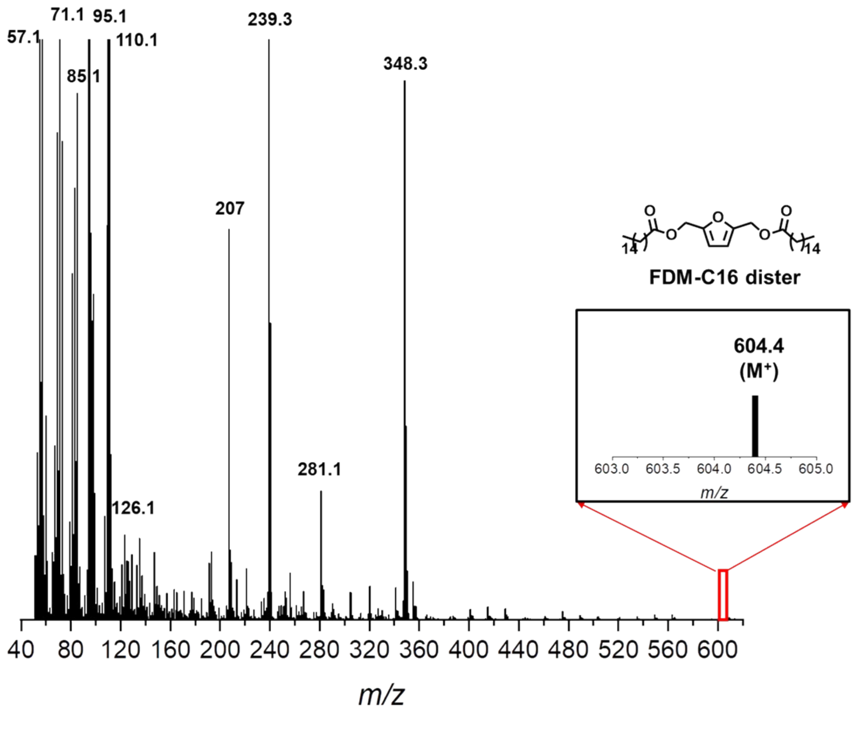

Figure S27. GC-MS total ion chromatogram (TIC) of purified **FDCA-C16** diester.

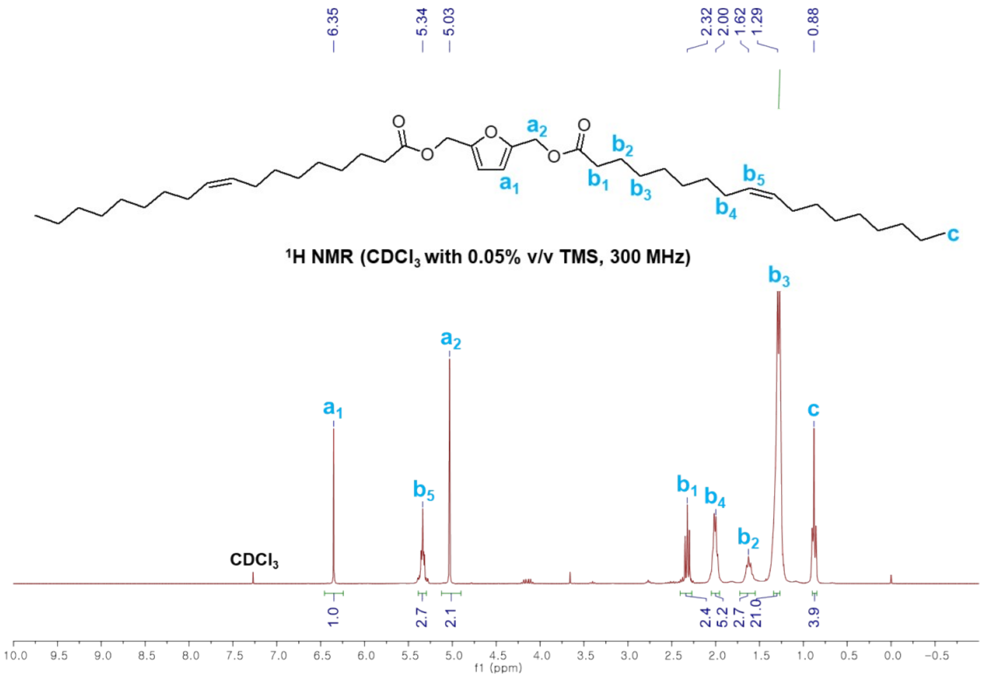

Figure S28. ¹H NMR spectrum (300 MHz, $CDCl_3$) of purified **FDM-C18** diester.

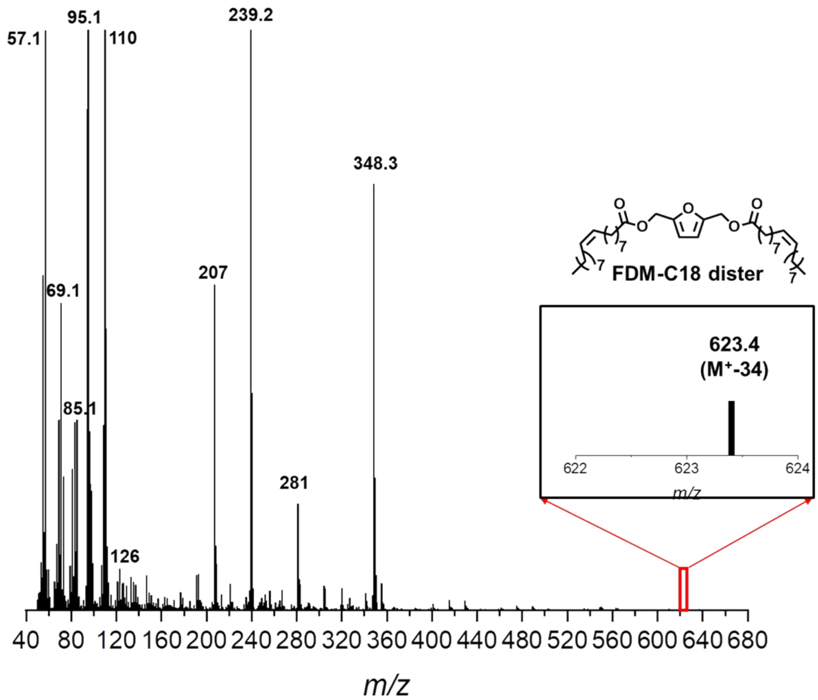

Figure S29. GC-MS total ion chromatogram (TIC) of purified **FDM-C18** diester.

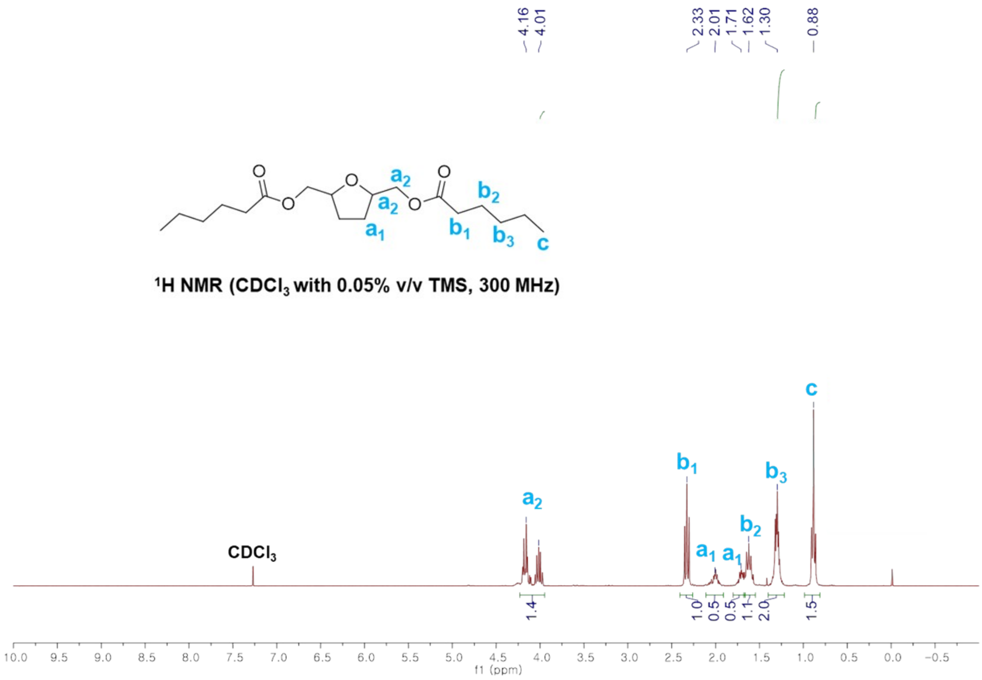

Figure S30. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDM-C6** diester.

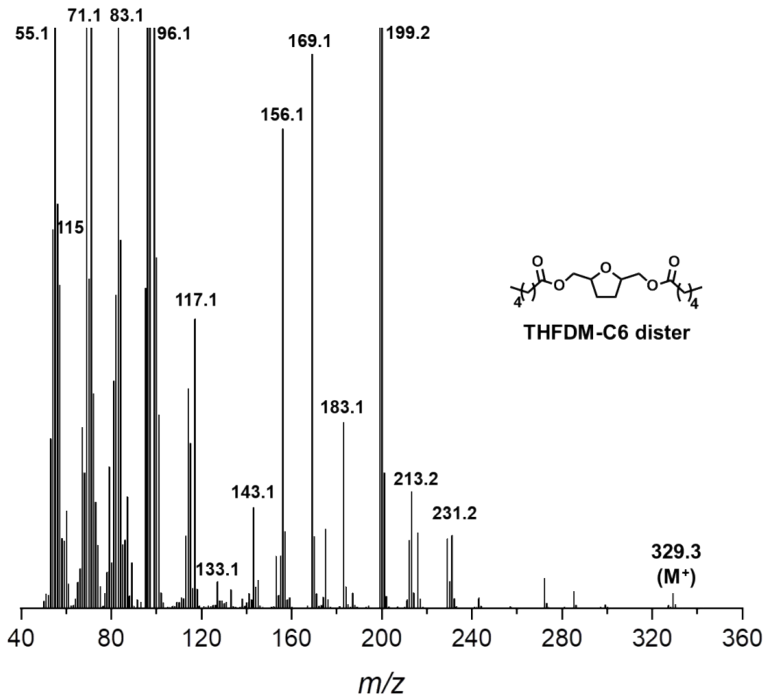

Figure S31. GC-MS total ion chromatogram (TIC) of purified **THFDM-C6** diester.

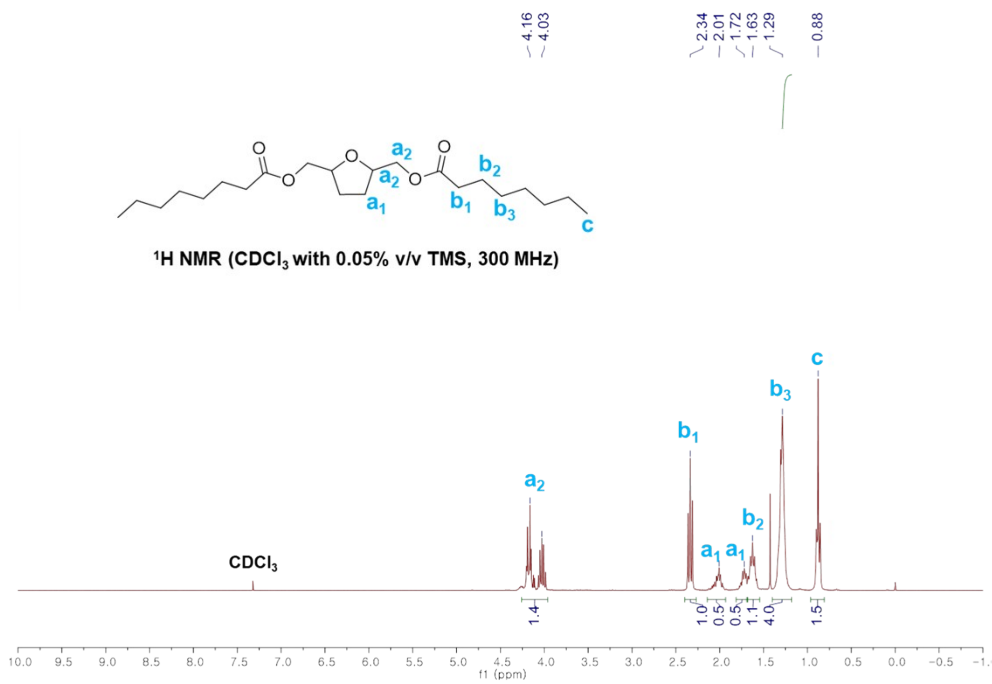

Figure S32. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDM-C8** diester.

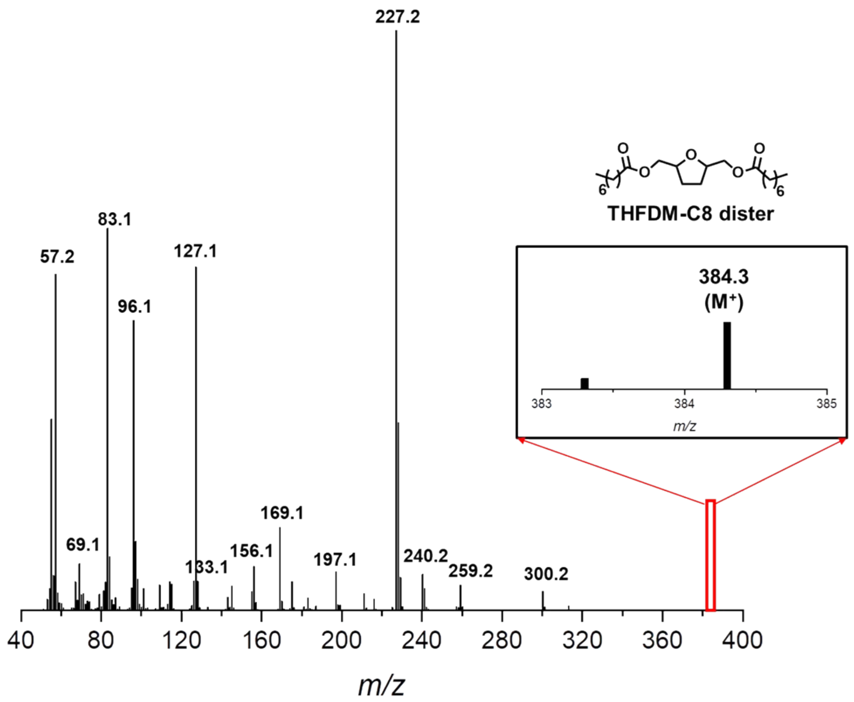

Figure S33. GC-MS total ion chromatogram (TIC) of purified **THFDM-C8** diester.

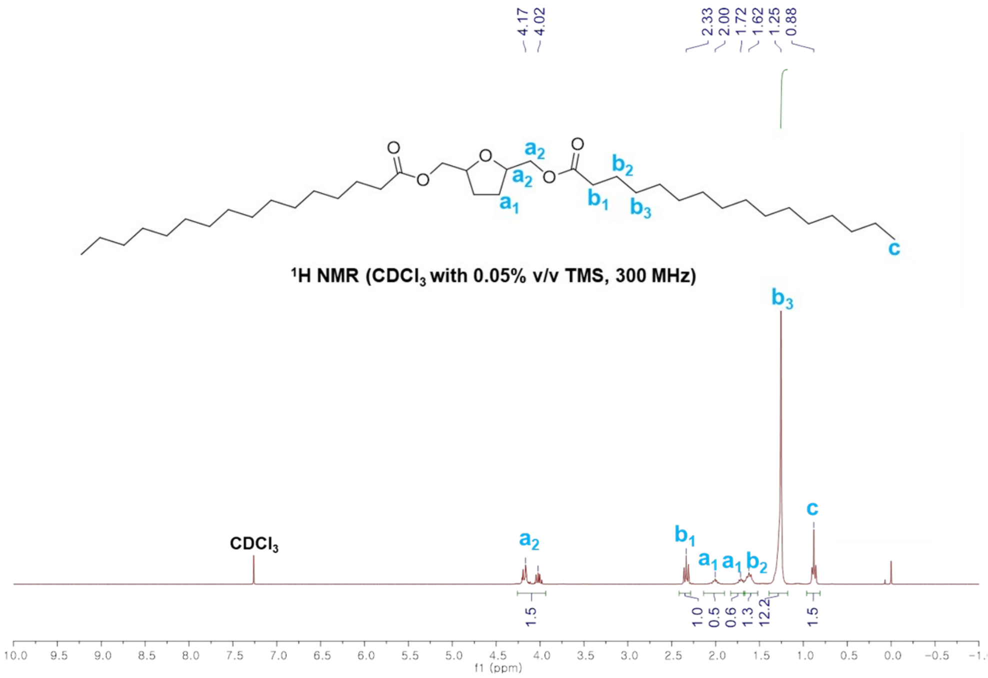

Figure S34. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDM-C16** diester.

Figure S35. GC-MS total ion chromatogram (TIC) of purified **THFDM-C16** diester.

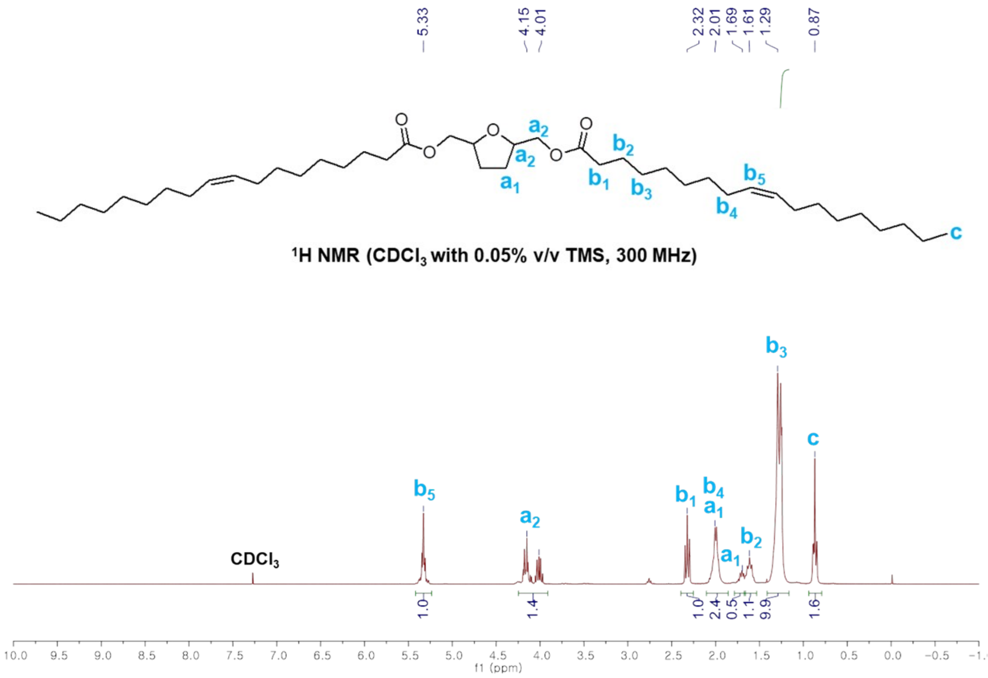

Figure S36. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of purified **THFDM-C18** diester.

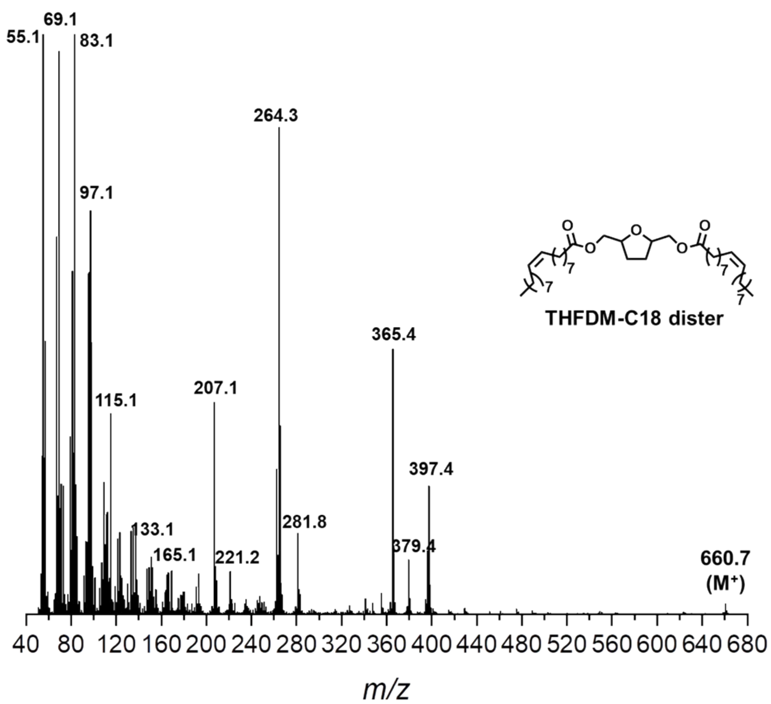

Figure S37. GC-MS total ion chromatogram (TIC) of purified **THFDM-C18** diester.

Table S1. Physical properties of the commercial lubricants

Products	KV (mm^2s^{-1})		VI	Pour point (°C)	Flashpoint (°C)
	KV_{40}	KV_{100}			
PAO2	5.2-8.8	1.7-2.8	-	<-50	>145
Combustion Engine Oil (SEA20) for Land Transport	-	5.6-9.3	>96	<-22.5	>80
Combustion Engine Oil (SAE20) for Land Transport	-	5.6-9.3	>75	<-12.5	>180
Combustion Engine Oil (SAE20) for Ship	-	5.6-9.3	>75	<-12.5	>190
Machine Oil (ISO VG32)	28.8-35.2	-	-	<-5	>150
Gear Oil (ISO VG32)	28.8-35.2	-	>90	<-10	>170
Gear Oil (SAE 80W)	-	>7.0	>85	<-20	>175
Turbine Oil (ISO VG32)	28.8-35.2	>4.2	-	<-7.5	>180
Bearing Oil (ISO VG10)	9.0-11.0	-	>80	<-5	>130
Bearing Oil (ISO VG32)	28.8-35.2	-	>90	<-5	>150
Auto Transmission Fluid	-	>5.5	>120	<-40	>170
Compressor Oil (VBL 32)	28.8-35.2	-	-	<9.0	>175
Working Fluid	28.8-35.2	-	>90	<-22.5	>170
Working Fluid (For Train)	-	6-8	>95	<-25	>210
Heat Transfer Oil (ISO VG10)	9.0-11.0	-	-	<-10	>130
Heat Transfer Oil (ISO VG32)	28.8-35.2	-	-	<-7.5	>150
Cutting Oil (hydrophobic)	>10	-	-	<-5	>130
Insulating Oil	<13	<4	-	<-27.5	>140
Corrosion Preventive Oil (KP-20-1)	>10	-	-	<-25.0	>115

Table S2. Detailed process simulation result data for HMF hydrogenation and THFDM purification.

	1	2	3	4	5	6	7	8	9	10	11	12
Temp. [ºC]	25	25	159.4	125.5	125.5	133.7	183.3	265.0	125.0	126.9	308.3	270.6
Pressure [bar]	1	1	41.4	1	1	1	1	1	1	41.4	1	1
H_2 [kg/h]	0	33.6	33.6	0	0	0	0	0	0	0	0	0
MEG [kg/h]	2571	0	36677	36677	30345	1517	121.4	7.8	2567	34106	0	3.9
5-HMF [kg/h]	733.5	0	733.5	0	0	0	0	0	0	0	0	0
Humins [kg/h]	0	0	0.1	32.4	32.4	32.3	32.3	32.3	0	0.1	28.7	3.5
THFDM [kg/h]	0	0	18.6	753.5	752.6	749.7	748.3	740.9	1.4	18.6	0.3	733.2

Table S3. Detailed process simulation result data for THFDM esterification and THFDM-C18 diester purification.

	13	**14**	**15**	**16**	**17**	**18**	**19**	**20**	**21**	**22**	**23**
Temp. [ºC]	25	149.9	149.9	149.9	386.3	406.6	442.7	475.8	95.7	357.4	518.7
Pressure [bar]	1	1	1	1	1	1	1	1	1	1	1
THFDM [kg/h]	733.2	738.1	8.1	8.0	5.0	0	0	0	3.2	5.0	0
Oleic acid [kg/h]	3017.8	4750.8	1770.7	1768.6	1768.6	1042.6	394.0	186.4	2.2	1733.0	35.6
Cyclohexane [kg/h]	1045.4	1045.4	1045.4	140.9	0.1	0	0	0	1045.4	0.1	0
H_2O [kg/h]	0	0	190.1	27.0	0	0	0	0	190.1	0	0
MO-C18[a] [kg/h]	0	33.2	230.4	230.4	230.4	228.1	223.5	219.0	0	33.2	197.1
DI-C18[b] [kg/h]	0	0	3322.9	3322.9	3322.9	3322.9	3322.9	3322.9	0	0	3322.9

[a]THFDM-C18 monoester, [b]THFDM-C18 diester

Table S4. Temperature and enthalpy values for HMF hydrogenation and THFDM purification by each heater/cooler.

Block		Inlet T (°C)	Outlet T (°C)	Enthalpy (MW)
H1(Heater)	Heat	115.43	159.85	1.047
D1(Reboiler)	Heat	133.17	133.67	7.73
D2(Reboiler)	Heat	182.75	183.25	1.72
D3(Reboiler)	Heat	264.47	264.97	0.54
D4(Reboiler)	Heat	307.80	308.30	0.13
D5(Reboiler)	Heat	270.11	270.61	0.02
H3(Heater)	Cool	125.02	124.70	0.86
R1(Reactor)	Cool	160.35	159.85	0.42
D1(Condenser)	Cool	125.51	125.01	7.73
D2(Condenser)	Cool	125.53	125.03	1.70
D3(Condenser)	Cool	126.74	126.24	0.50
D4(Condenser)	Cool	264.16	263.66	0.13
D5(Condenser)	Cool	150.96	150.46	0.02

Table S5. Temperature and enthalpy values for THFDM esterification and THFDM-C18 diester purification by each heater/cooler.

Block		Inlet T (°C)	Outlet T (°C)	Enthalpy (MW)
H2(Heater)	Heat	132.15	149.85	0.10
R2(Heater)	Heat	149.35	149.85	1.70
D6(Reboiler)	Heat	385.79	386.29	0.95
D7(Reboiler)	Heat	406.09	406.59	0.61
D8(Reboiler)	Heat	442.19	442.69	0.58
D9(Reboiler)	Heat	475.35	475.85	0.35
D10(Reboiler)	Heat	518.21	518.71	0.40
D6(Condenser)	Cool	90.62	90.12	0.10
D7(Condenser)	Cool	351.70	351.20	0.56
D8(Condenser)	Cool	362.20	361.70	0.50
D9(Condenser)	Cool	362.57	362.07	0.27
D10(Condenser)	Cool	365.57	365.07	0.29

Table S6. Temperature and heat capacity values of energy utility streams

Utility Stream		Inlet T (°C)	Outlet T (°C)	C_p (KJ/kg/°C)
LLP Steam	Heat	147.6	146.6	2121.2
LP Steam	Heat	185.5	184.5	1994.3
MP Steam	Heat	237.5	236.5	1777.4
HP Steam	Heat	386.0	385.0	1686.9
Mineral Oil	Heat	600.0	599.0	206.0
Cooling Water	Cool	25	35	4.3

Table S7. Project cost worksheet including total direct cost and total capital investment for THFDM production and THFDM-C18 production.

Capital cost estimation			**Installed costs**
THFDM production			$36,850,400
THFDM-C18 diester production			$16,929,000
Heat and power generation			$16,926,220
HEN			$1,387,037
Storage			$949,410
Total Installed cost			$73,042,067
Warehouse	4.0%	of *ISBL	$2,151,176
Site development	9.0%	of *ISBL	$4,840,146
Additional piping	4.5%	of *ISBL	$2,420,073
Total direct cost (TDC)			$82,453,462
Prorateable expenses	10.0%	of TDC	$8,245,346
Field expenses	10.0%	of TDC	$8,245,346
Home office & construction fee	20.0%	of TDC	$16,490,692
Project contingency	10.0%	of TDC	$8,245,346
Other costs (Start-Up, Permits, etc.)	10.0%	of TDC	$8,245,346
Total indirect cost			$49,472,077
Fixed capital investment (FCI)			$131,925,539
Land	1.5%	of TCI	$2,109,469
Working capital	5.0%	of FCI	$6,596,277
Total capital investment (TCI)			**$140,631,285**

*Inside-battery-limits (ISBL) equipment costs include THFDM production and THFDM-C18 diester production.

Table S8. Discounted cashflow sheet of THFDM production and THFDM-C18 diester production (part 1)

Year	-2	-1	0	1	2	3	4	5	6	7	8
Capital Investment	4,221,617	31,662,129	16,886,469								
Land	2,109,469										
Working Capital			6,596,277								
Loan payment				11,796,477	11,796,477	11,796,477	11,796,477	11,796,477	11,796,477	11,796,477	11,796,477
Loan interest payment	506,594	4,306,050	6,332,426	6,332,426	5,895,302	5,423,208	4,913,346	4,362,696	3,767,993	3,125,714	2,432,053
Loan principal	6,332,426	53,825,620	79,155,323	73,691,272	67,790,096	61,416,826	54,533,695	47,099,913	39,071,429	30,400,666	21,036,242
THFDM-C18 diester				128,639,909	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039
Excess electricity				1,353,106	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407
Total Annual Sales				129,993,015	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446
Feed cost				31,089,924	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342
Variable Operating Costs				71,178,082	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287
Fixed Operating Costs				6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859
Total Product Cost				108,320,864	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488
Annual Depreciation											
General Plant											
MACRS method (7yr)				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%
Depreciation Charge				16,433,403	28,163,333	20,113,381	14,363,415	10,269,439	10,257,939	10,269,439	5,128,970
Remaining Value				98,565,916	70,402,583	50,289,202	35,925,787	25,656,348	15,398,409	5,128,970	0
Power and Steam Plant											
MACRS method (20yr)				3.75%	7.22%	6.68%	6.18%	5.71%	5.29%	4.89%	4.52%
Depreciation Charge				634,733	1,221,904	1,130,164	1,045,533	966,995	894,551	827,354	765,404
Remaining Value				16,291,486	15,069,583	13,939,419	12,893,886	11,926,891	11,032,341	10,204,987	9,439,583
Remaining Value				114,857,403	85,472,166	64,228,621	48,819,674	37,583,240	26,430,750	15,333,957	9,439,583
Net Revenue				-1,728,411	-4,224,581	4,389,206	10,733,664	15,456,828	16,135,475	16,833,451	22,729,531
Losses Forward					-1,728,411	-5,952,992	-1,563,786	0	0	0	0
Taxable Income				-1,728,411	-5,952,992	-1,563,786	9,169,878	15,456,828	16,135,475	16,833,451	22,729,531
Income Tax				0	0	0	3,209,457	5,409,890	5,647,416	5,891,708	7,955,336
Annual Cash Flow				9,875,673	19,259,481	19,259,481	16,050,023	13,849,591	13,612,064	13,367,773	11,304,145
Discount Factor	1.3225	1.1500	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269
Annual Present Value				8,587,542	14,562,934	12,663,421	9,176,653	6,885,694	5,884,871	5,025,441	3,695,345
TPI + Interest	9,042,833	41,363,406	29,815,172	5,506,457	4,457,695	3,565,847	2,809,222	2,169,031	1,629,007	1,175,072	795,043
NPV			0								

Table S9. Discounted cashflow sheet of THFDM production and THFDM-C18 diester production (part 2)

Year	9	10	11	12	13	14	15	16	17	18	19
Capital Investment											
Land											
Working Capital											
Loan payment	11,796,477	11,796,477									
Loan interest payment	1,682,899	873,813									
Loan principal	10,922,664	0									
THFDM-C18 diester	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039
Excess electricity	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407
Total Annual Sales	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446
Feed cost	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342
Variable Operating Costs	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287
Fixed Operating Costs	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859
Total Product Cost	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488
Annual Depreciation											
General Plant											
MACRS method (7yr)											
Depreciation Charge											
Remaining Value											
Power and Steam Plant											
MACRS method (20yr)	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%
Depreciation Charge	755,248	755,079	755,248	755,079	755,248	755,079	755,248	755,079	755,248	755,079	755,248
Remaining Value	8,684,336	7,929,257	7,174,009	6,418,930	5,663,682	4,908,604	4,153,356	3,398,277	2,643,029	1,887,951	1,132,703
Remaining Value	8,684,336	7,929,257	7,174,009	6,418,930	5,663,682	4,908,604	4,153,356	3,398,277	2,643,029	1,887,951	1,132,703
Net Revenue	28,617,811	29,427,066	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710
Losses Forward	0	0	0	0	0	0	0	0	0	0	0
Taxable Income	28,617,811	29,427,066	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710	30,300,879	30,300,710
Income Tax	10,016,234	10,299,473	10,605,249	10,605,308	10,605,249	10,605,308	10,605,249	10,605,308	10,605,249	10,605,308	10,605,249
Annual Cash Flow	9,243,247	8,960,007	20,450,709	20,450,650	20,450,709	20,450,650	20,450,709	20,450,650	20,450,709	20,450,650	20,450,709
Discount Factor	0.2843	0.2472	0.2149	0.1869	0.1625	0.1413	0.1229	0.1069	0.0929	0.0808	0.0703
Annual Present Value	2,627,508	2,214,777	4,395,741	3,822,373	3,323,812	2,890,263	2,513,279	2,185,454	1,900,400	1,652,517	1,436,976
TPI + Interest	478,385	215,993	0	0	0	0	0	0	0	0	0
NPV											

Table S10. Discounted cashflow sheet of THFDM production and THFDM-C18 diester production (part 3)

Year	20	21	22	23	24	25	26	27	28	29	30
Capital Investment											
Land											-2,109,469
Working Capital											-6,596,277
Loan payment											
Loan interest payment											
Loan principal											
THFDM-C18 diester	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039	147,017,039
Excess electricity	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407	1,546,407
Total Annual Sales	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446	148,563,446
Feed cost	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342	35,531,342
Variable Operating Costs	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287	75,923,287
Fixed Operating Costs	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859	6,052,859
Total Product Cost	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488	117,507,488
Annual Depreciation											
General Plant											
MACRS method (7yr)											
Depreciation Charge											
Remaining Value											
Power and Steam Plant											
MACRS method (20yr)	4.46%	2.23%									
Depreciation Charge	755,079	377,624									
Remaining Value	377,624	0									
Remaining Value	377,624	0									
Net Revenue	30,300,879	30,678,334	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958
Losses Forward	0	0	0	0	0	0	0	0	0	0	0
Taxable Income	30,300,879	30,678,334	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958	31,055,958
Income Tax	10,605,308	10,737,417	10,869,585	10,869,585	10,869,585	10,869,585	10,869,585	10,869,585	10,869,585	10,869,585	10,869,585
Annual Cash Flow	20,450,650	20,318,541	20,186,373	20,186,373	20,186,373	20,186,373	20,186,373	20,186,373	20,186,373	20,186,373	20,186,373
Discount Factor	0.0611	0.0531	0.0462	0.0402	0.0349	0.0304	0.0264	0.0230	0.0200	0.0174	0.0151
Annual Present Value	1,249,540	1,079,538	932,622	810,976	705,196	613,214	533,230	463,678	403,198	350,607	304,876
TPI + Interest	0	0	0	0	0	0	0	0	0	0	-131,483
NPV											

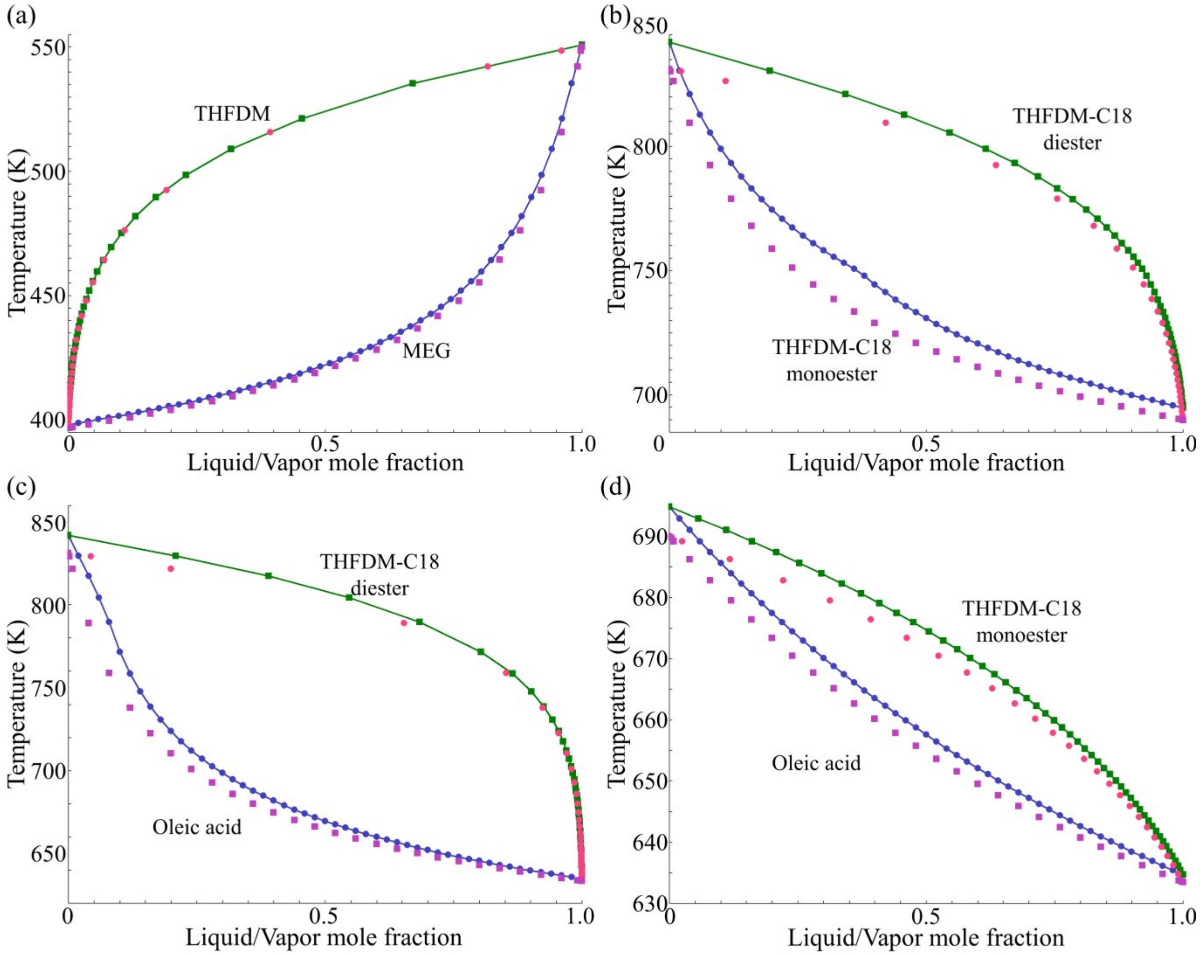

Figure S38. T-xy diagrams for the calculated VLE data (dot) and fitting VLE data (line) of the binary system. (a) THFDM and MEG, (b) THFDM-C18 monoester and THFDM-C18 diester, (c) Oleic acid and THFDM-C18 diester, and (d) Oleic acid and THFDM-C18 monoester.

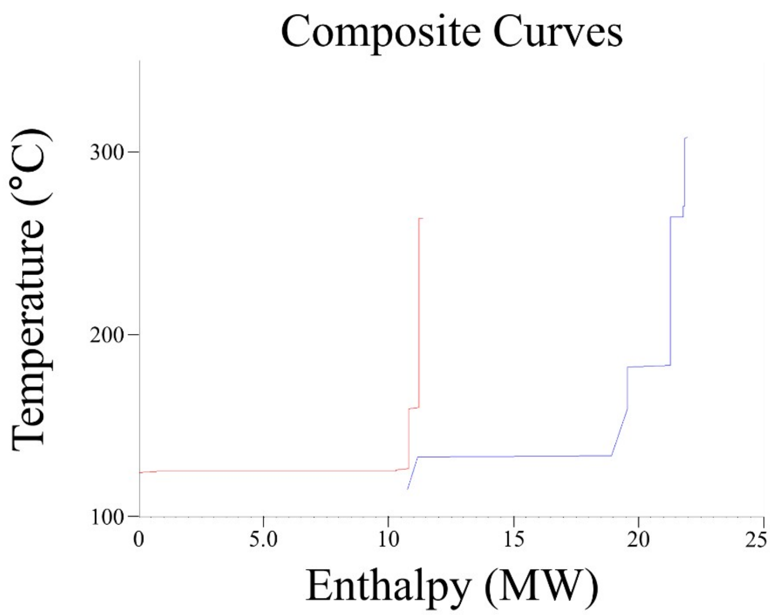

Figure S39. Composite curve of HMF hydrogenation and THFDM purification using Aspen Energy Analyzer

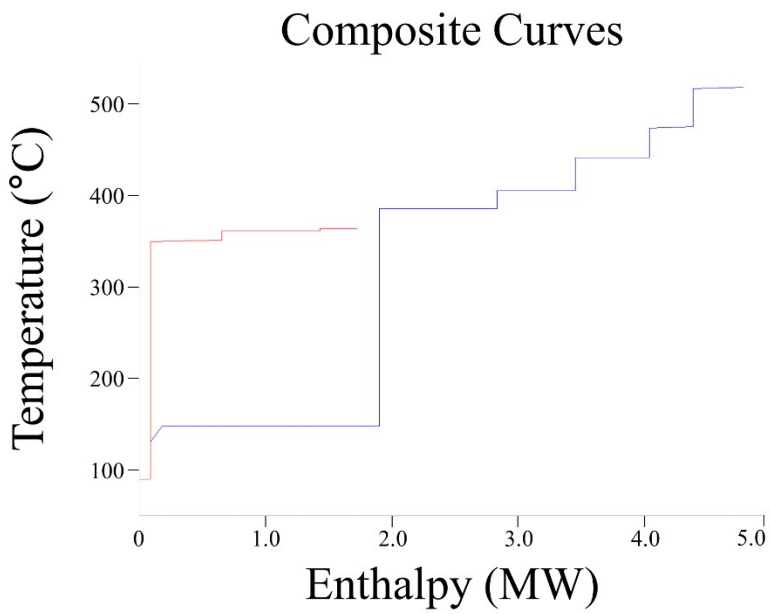

Figure S40. Composite curve of THFDM esterification and THFDM-C18 diester purification using Aspen Energy Analyzer

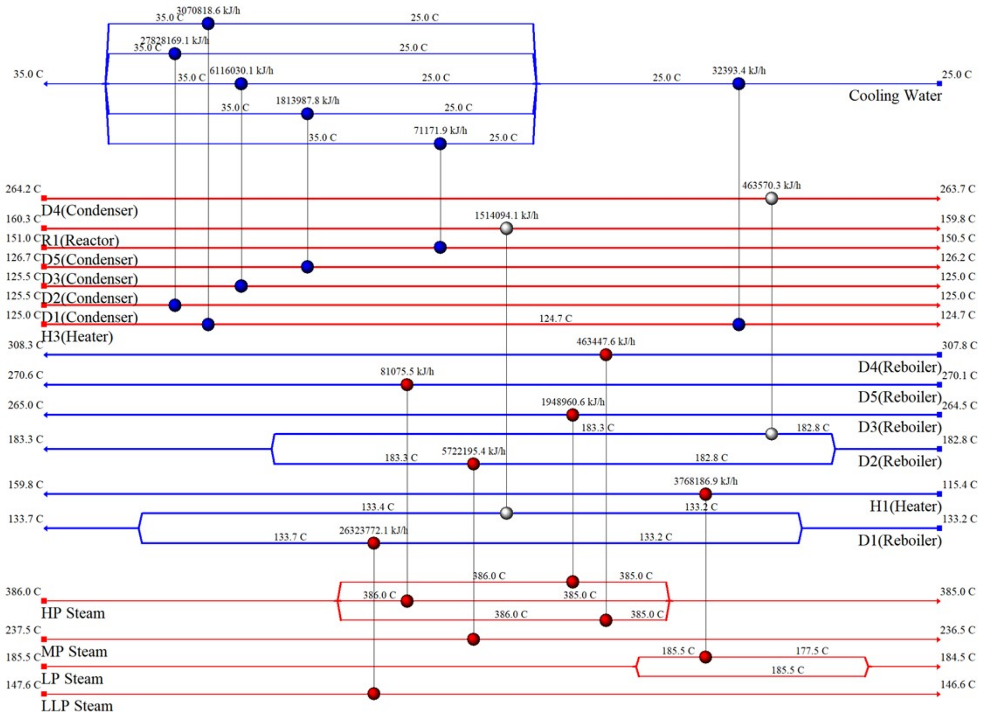

Figure S41. The suggested heat exchanger network for HMF hydrogenation and THFDM purification process, obtained using Aspen Energy Analyzer (minimum temperature difference, ΔTmin is 10 K).

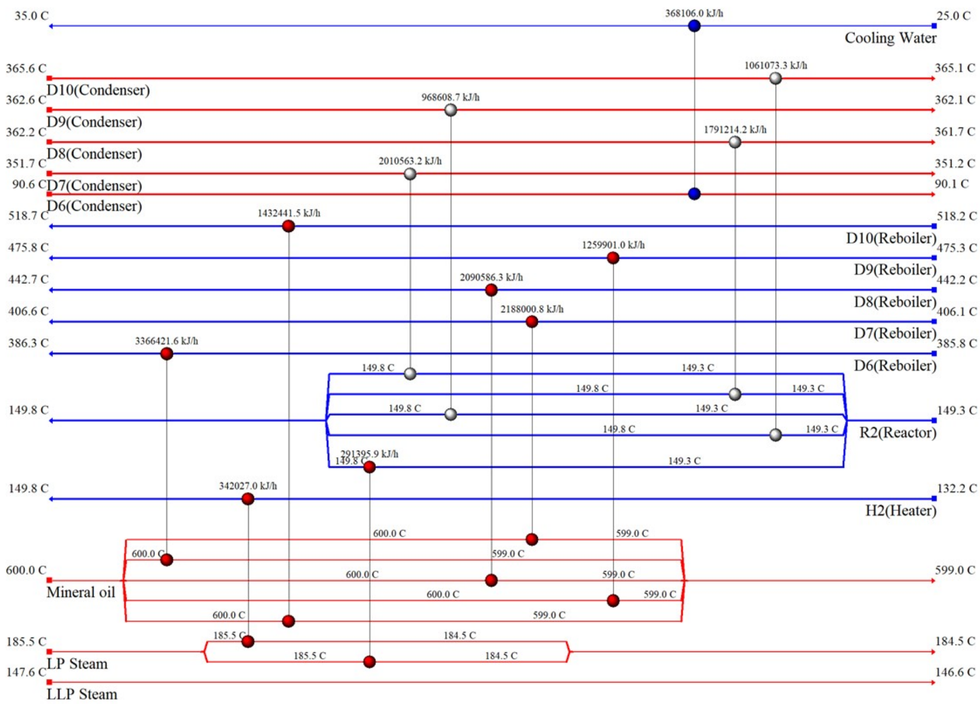

Figure S42. The suggested heat exchanger network for THFDM esterification and THFDM-C18 diester purification process, obtained using Aspen Energy Analyzer (minimum temperature difference,

ΔTmin is 10 K).

Reference

1. S. Prahlada Rao and S. Sunkada, *Resonance*, 2007, **12**, 43-57.