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Supporting Information

Separation of Saturated Fatty Acids and Fatty Acid Methyl Esters with Epoxy Nanofiltration Membranes Chad M. Gilmer, Christina Zvokel, Alexandra Vick and Ned B. Bowden Department of Chemistry University of Iowa, Iowa City, IA, 52242 ned-bowden@uiowa.edu

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Permeation of fatty acids through an epoxy membrane in a diffusion apparatus.



Fig S1. Diffusion apparatus used to monitor the flux of FAs and FAMEs through the epoxy membrane.

Table S1. Initial screening of the permeation of model fatty acids through epoxy mer	nbranes.
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Molecules	Membrane	Relative Flux	Normalized
			Flux
			(mol/cm ² *h) ^a
Butyric Acid		5.84	2.83 x 10 ⁻⁶
Undecylenic Acid	A-1	1.75	8.49 x 10 ⁻⁷
Stearic Acid		1	4.85 x 10 ⁻⁷
Butyric Acid		7.02	9.90 x 10 ⁻⁷
Undecylenic Acid	A-2	3.01	4.24 x 10 ⁻⁷
Stearic Acid		1.00	1.41 x 10 ⁻⁷
Butyric Acid		21.4	4.24 x 10 ⁻⁷
Undecylenic Acid	A-3	4.29	8.49 x 10⁻ ⁸
Stearic Acid		1.00	1.98 x 10 ⁻⁸

^aAll flux values carry a ± 4.24% relative error.

Molecule	Membrane	Relative Flux	Normalized Flux (mol/cm ² *h) ^a
Butyric acid		7.97	1.41 x 10 ⁻⁶
Undecylenic acid	A-1 ³ 3 ¹	3.20	5.66 x 10 ⁻⁷
Stearic acid		1.00	1.77 x 10 ⁻⁷
Butyric acid		16.6	1.41 x 10 ⁻⁶
Undecylenic acid	A-1 ¹ 3 ¹	4.99	4.24 x 10 ⁻⁷
Stearic acid		1.00	8.49 x 10 ⁻⁸
Butyric acid		22.5	8.49 x 10 ⁻⁷
Undecylenic acid	A-1 ¹ 3 ³	7.51	2.83 x 10 ⁻⁷
Stearic acid		1.00	3.77 x 10 ⁻⁸

Table S2. Permeation of model fatty acids through epoxy membranes fabricated with epoxides1 and 3.

^aAll flux values carry a ± 4.24% relative error.

Table S3. Permeation of model fatty acids through epoxy membranes fabricated with epoxides2 and 3.

Molecule	Membrane	Relative Flux	Normalized Flux (mol/cm ² *h) ^a
Butyric acid		30.0	8.49 x 10 ⁻⁷
Undecylenic acid	A-2 ³ 3 ¹	4.98	1.41 x 10 ⁻⁷
Stearic acid		1.00	2.83 x 10 ⁻⁸
Butyric acid		20.0	8.49 x 10 ⁻⁷
Undecylenic acid	A-2 ¹ 3 ¹	3.33	1.41 x 10 ⁻⁷
Stearic acid		1.00	4.24 x 10 ⁻⁸
Butyric acid		60.2	8.49 x 10 ⁻⁷
Undecylenic acid	A-2 ¹ 3 ³	8.01	1.13 x 10 ⁻⁷
Stearic acid		1.00	1.41 x 10 ⁻⁸

^aAll flux values carry a ± 4.24% relative error.

Molecule	Membrane	Relative Flux	Normalized Flux (mol/cm ² *h) ^a
		6.67	2.83×10^{-6}
Butyric acid		6.67	
Undecylenic acid	A-1 ¹ 2 ³	3.00	1.27 x 10⁻ ⁶
Stearic acid		1.00	4.24 x 10 ⁻⁷
Butyric acid		4.99	4.24 x 10 ⁻⁶
Undecylenic acid	A-1 ¹ 2 ¹	1.67	1.41 x 10 ⁻⁶
Stearic acid		1.00	8.49 x 10 ⁻⁷
Butyric acid		6.67	3.77 x 10 ⁻⁶
Undecylenic acid	A-1 ³ 2 ¹	3.00	1.70 x 10 ⁻⁶
Stearic acid		1.00	5.66 x 10 ⁻⁷

Table S4. Permeation of model fatty acids through epoxy membranes fabricated with epoxides1 and 2.

^aAll flux values carry a ± 4.24% relative error.

Permeation of fatty acid methyl esters (FAMEs) through a membrane in a diffusion apparatus.

Table S5. Permeation of saturated FAMEs through membrane A-2¹3³

Molecule	Relative Flux	Normalized Flux (mol/cm ² *h) ^a
Methyl butyrate (C ₄)	100	9.90 x 10 ⁻⁸
Methyl hexanoate (C ₆)	57.1	5.66 x 10 ⁻⁸
Methyl octanoate (C ₈)	28.6	2.83 x 10 ⁻⁸
Methyl decanoate (C ₁₀)	14.3	1.41 x 10 ⁻⁸
Methyl laurate (C ₁₂)	8.58	8.49 x 10 ⁻⁹
Methyl myristate (C ₁₄)	4.28	4.24 x 10 ⁻⁹
Methyl palmiate (C ₁₆)	2.86	2.83 x 10 ⁻⁹
Methyl stearate (C ₁₈)	1.00	9.90 x 10 ⁻¹⁰

^aAll flux values carry a ± 4.24% relative error.

Molecule	Relative Flux	Normalized Flux
		(mol/cm ² *h) ^a
Methyl butyrate (C ₄)	49.8	1.41 x 10 ⁻⁷
Methyl hexanoate (C ₆)	28.3	8.49 x 10⁻ ⁸
Methyl octanoate (C ₈)	18.9	5.66 x 10⁻ ⁸
Methyl decanoate (C ₁₀)	10.0	2.83 x 10⁻ ⁸
Methyl laurate (C ₁₂)	4.70	1.41 x 10⁻ ⁸
Methyl myristate (C ₁₄)	3.50	9.90 x 10 ⁻⁹
Methyl palmiate (C ₁₆)	1.89	5.66 x 10 ⁻⁹
Methyl stearate (C ₁₈)	1.00	2.83 x 10⁻ ⁹

Table S6. Permeation of saturated FAMEs through membrane A-1¹3³

^aAll flux values carry a \pm 4.24% relative error.

¹H NMR and ¹³C NMR spectrums of methyl undecylenate.

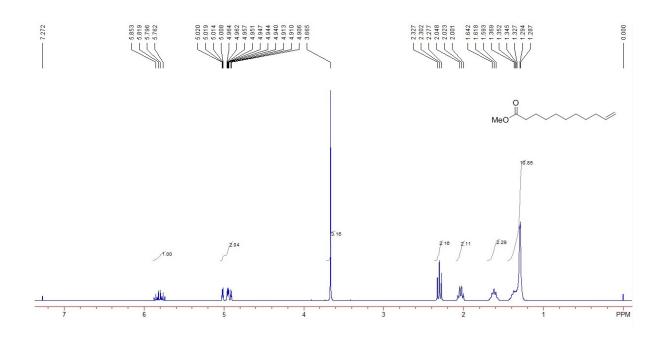


Figure S2. ¹H NMR spectrum of methyl undecylenate in CDCl₃.

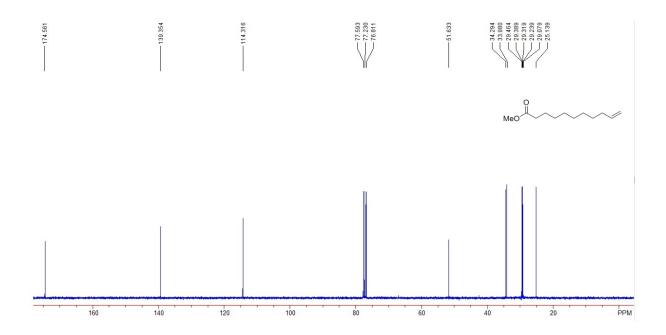


Figure S3. ¹³C NMR spectrum of methyl undecylenate in CDCl₃.

AFM images of spin-coated epoxy membrane A-2.

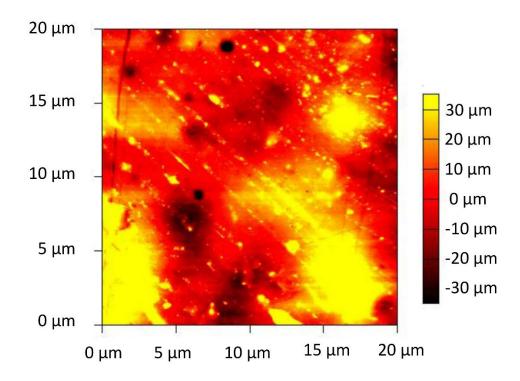


Figure S4. 2D AFM image showing the changes in height on the surface of a spin-coated epoxy membrane A-2.

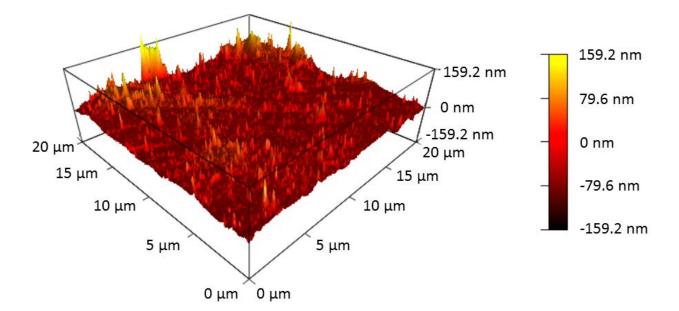


Figure S5. 3D AFM image showing the changes in height on the surface of a spin-coated epoxy membrane.

Permeation of methyl undecylenate and methyl stearate through membrane A-2 in a pressure apparatus.

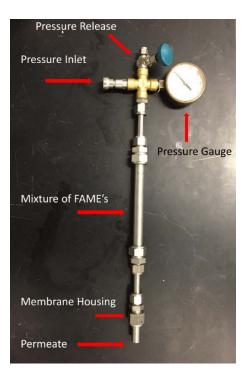


Figure S6. Dead end-filtration apparatus for high pressure experiments

	Mass of FAMEs (mg)	Methyl Undecylenate (mol%)	Methyl Stearate (mol %)
Initial ^a	1,860	49.9	50.1
Fraction 1	38.0	67.9	32.1
Fraction 2	42.3	68.5	31.5
Fraction 3	44.3	67.7	32.3
Fraction 4	85.1	70.0	30.0
Fraction 5 ^b	60.7	62.2	37.8
Total Permeate	270	67.4	32.6
Retention	1,480	45.5	54.5

Table S7. Composition of FAMEs collected in the pressure experiment with membrane A-2.

^aInitial composition was determined by removing a 1 mL sample of the initial mixture and analyzing via ¹H NMR spectroscopy.

^bFraction 5 is the sample that was on the permeate side of the dead-end filtration and did not go into the vial. This sample was collected by washing the end of the metal apparatus with DCM and removing DCM to obtain the FAMEs.

Table S8. Composition of FAME's collected in the pressure experiment with membrane A-2 ¹ 3 ³ .

	Mass of	Methyl	Methyl	Ethyl Stearate ^d
	FAME's and	, Hexanoate	Undecylenate	, (mol%)
	FAEE (mg)	(mol%)	(mol%)	
Initial ^a	2,380	32.8	33.1	34.1
Fraction 1	12.0	17.7 ^c	62.1	20.2
Fraction 2 ^b	53.6	30.6 ^c	52.5	16.8
Retention	2,110	32.3	32.2	35.4

^aInitial composition was determined by removing a 1 mL sample of the initial mixture and analyzing via ¹H NMR spectroscopy.

^bFraction 2 is the sample that was on the permeate side of the dead-end filtration and did not go into the vial. This sample was collected by washing the end of the metal apparatus with DCM and removing DCM to obtain the FAMEs.

^cDue to the low boiling point of methyl hexanoate, it had evaporated from the permeate side before analysis could be completed.

^dEthyl stearate was used in this experiment because it has a unique peak in the ¹H NMR spectrum that so it can be distinguished from the other two FAMEs being used.

Permeation of a multicomponent mixture of FAMEs through epoxy membrane A-2 in a pressure apparatus.

	Mass of	Methyl	Methyl	Methyl	Methyl	Methyl
	FAMEs	Decanoate	Laurate	Myristate	Palmitate	Stearate
	(mg)	(mol%)	(mol %)	(mol%)	(mol%)	(mol%)
Initial	4,510	23.2	20.6	19.7	19.6	16.8
Fraction 1	46.1	31.0	21.5	18.9	15.5	13.0
Fraction 2	10.2	31.8	21.6	17.6	16.3	12.7
Fraction 3	53.7	31.1	23.2	18.5	15.2	12.0
Fraction 4	91.8	30.9	24.1	18.5	15.4	11.0
Fraction 5 ^b	85.5	27.7	24.9	19.0	16.5	11.9
Total Permeate	287	30.3	23.4	18.6	15.8	11.9
Retention	3,920	22.1	22.0	19.7	20.1	16.1

Table S9. Composition of FAMEs collected in the pressure experiment with membrane A-2.

^a Initial composition was determined by removing a 1 mL sample of the initial mixture and analyzing via gas chromatography-mass spectrometry (GC-MS).

^bFraction 5 is the sample that was on the permeate side of the dead-end filtration and did not go into the vial. This sample was collected by washing the end of the metal apparatus with DCM and removing DCM to obtain the FAMEs.