

# **Simultaneous Extraction, Fractionation and Enrichment of Microalgal Triacylglycerides by Exploiting the Tunability of Neat Supercritical Carbon Dioxide**

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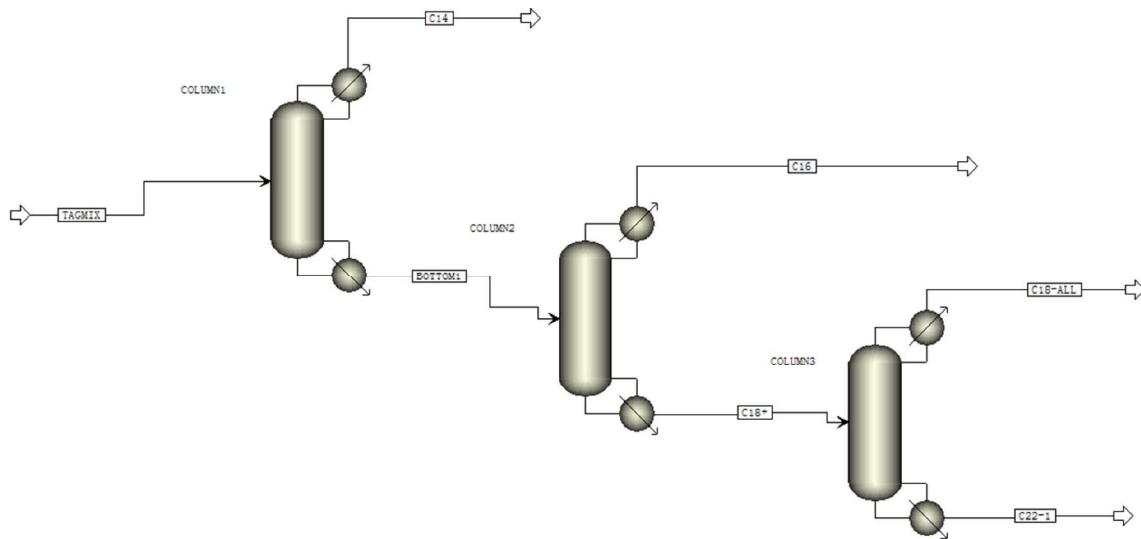
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This six page supplement contains the following materials:

Figure S.1 Process flow diagram (PFD) of the downstream processing model

Table S.2 Operating conditions and solubilities of analytical standard and *Chlorella* sp. TAG extracts

Table S.3 Solubility separation factors



**Figure S.1** Process flow diagram (PFD) for the downstream processing model

**Table S.2** Measured solubility,  $y^*$ , and operational conditions for binary and multi-component analytical standard TAG mixtures and TAGs extracted from the microalgae *Chlorella* sp. (Note: extracts from *Chlorella* sp. were modeled to be a triacylglyceride with identical fatty acids and reported as the modeled chain length and saturation.)

	<i>T</i> °C	<i>P</i> MPa	Density mg/mL	$y^*$ solute/solvent	<i>R</i> <sup>2</sup>	<i>stdev</i>
Binary Mixture of Analytical Standards						
C16:0	40	8.31	384	0.02	0.983	7.9E-03
C18:1			(very low)	0.06	0.999	1.3E-03
Multi-component Mixture of Analytical Standards						
Unsaturated MUFA	C14:0			0.06	0.997	1.9E-03
	C16:0			0.04	0.923	9.3E-03
	C18:0	40	550	0.03	0.945	5.3E-03
	C16:1	9.3	(medium)	0.11	0.987	1.6E-03
	C18:1			0.05	0.995	1.4E-03
	C20:1			0.11	0.996	1.3E-03
	Unsaturated	C14:0	40	750	0.11	0.989
		C16:0	13.35	(high)	0.07	0.951

	C18:0		0.09	0.980	1.7E-03	
MUFA	C16:1		0.05	0.925	9.2E-03	
	C18:1		0.05	0.956	7.4E-03	
	C20:1		0.16	0.993	2.7E-03	
Unsaturated	C14:0		0.17	0.968	2.8E-03	
	C16:0		0.43	0.984	1.3E-02	
	C18:0	40      17.2	812 <i>(very high)</i>	0.21	0.963	5.2E-03
MUFA	C16:1		0.11	0.982	5.2E-03	
	C18:1		0.14	0.978	3.4E-03	
	C20:1		0.54	0.929	1.3E-02	
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<i>Chlorella</i> sp.						
Unsaturated	C14:0		0.01	0.977	7.2E-03	
	C16:0		0.18	0.994	2.3E-02	
	C18:0		0.04	0.994	6.3E-03	
MUFA	C20:0		<0.01	0.964	7.5E-03	
	C22:0	37      8.3	463 <i>(low)</i>	0.01	0.992	5.9E-03
	C16:1		0.01	0.987	6.8E-03	
PUFA	C18:1		0.01	0.982	6.3E-03	
	C18:2		0.01	0.979	7.4E-03	
	C18:3		<0.01	0.972	7.1E-03	
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Unsaturated	C14:0		0.01	0.924	6.0E-03	
	C16:0		0.17	0.825	3.6E-02	
	C18:0		0.07	0.926	1.2E-02	
MUFA	C20:0		0.08	0.909	2.3E-02	
	C22:0		<0.01	0.828	3.4E-03	
	C24:0	60      13.8	556 <i>(medium)</i>	<0.01	0.907	8.7E-04
PUFA	C16:1		0.02	0.913	6.2E-03	
	C18:1		0.15	0.956	3.0E-02	
	C22:1		<0.01	0.715	1.2E-05	
PUFA	C18:2		0.10	0.996	1.9E-02	
	C18:3		0.02	0.919	5.7E-03	
Unsaturated	C14:0		<0.01	0.803	7.8E-04	
	C16:0		0.16	0.981	2.3E-02	
	C18:0		0.03	0.979	8.7E-03	
MUFA	C20:0	40      13.4	750 <i>(high)</i>	0.01	0.988	1.5E-03
	C24:0		0.07	0.810	4.1E-02	
	C16:1		0.14	0.998	2.5E-02	
MUFA	C18:1		0.25	0.999	2.4E-02	
	C22:1		0.01	0.984	3.0E-03	

PUFA	C18:2		0.15	0.999	2.4E-02
	C18:3		0.17	0.993	3.2E-02

**Table S.3** Solubility separation factors for 6-component analytical standard and *chlorella* sp. extracts at very low, low, medium, high and very high scCO<sub>2</sub> densities.

CO <sub>2</sub> Density	Multi-Component		
	medium	high	very high
	550 mg/ml	750 mg/ml	812 mg/ml
C14:0/C16:0	1.54	1.53	0.40
C14:0/C16:1	0.52	2.15	1.58
C14:0/C18:0	2.10	1.29	0.80
C14:0/C18:1	1.06	2.18	1.18
C14:0/C20:1	0.49	0.71	0.31
C16:0/C16:1	0.34	1.40	3.99
C16:0/C18:0	1.37	0.84	2.02
C16:0/C18:1	0.69	1.42	2.98
C16:0/C20:1	0.32	0.46	0.79
C16:1/C18:0	4.06	0.60	0.51
C16:1/C18:1	2.04	1.02	0.67
C16:1/C20:1	0.94	0.33	0.20
C18:0/C18:1	0.50	1.69	1.48
C18:0/C20:1	0.23	0.55	0.39
C18:1/C20:1	0.46	0.33	0.26

CO <sub>2</sub> Density	<i>Chlorella</i> sp.		
	low	medium	high
	463 mg/ml	556 mg/ml	750 mg/ml
C14:0/C16:0	0.07	0.03	0.01
C14:0/C16:1	0.62	1.14	0.01
C14:0/C18:0	0.19	0.17	0.05
C14:0/C18:1	0.08	0.42	0.01
C14:0/C18:2	0.12	0.61	0.01
C14:0/C18:3	0.69	2.16	0.01
C14:0/C20:0	0.16	2.36	0.36
C14:0/C22:0	3.91	0.87	0.19
C14:0/C22:1	-	4.51	0.21
C14:0/C24:0	-	3.53	0.03
C16:0/C16:1	8.30	34.32	1.12

C16:0/C18:0	2.52	4.97	4.65
C16:0/C18:1	1.08	12.77	0.65
C16:0/C18:2	1.59	18.45	1.05
C16:0/C18:3	9.18	65.08	0.96
C16:0/C20:0	2.14	71.08	30.54
C16:0/C22:0	52.40	26.10	16.29
C16:0/C22:1	-	135.72	17.53
C16:0/C24:0	-	106.08	2.32
C16:1/C18:0	0.30	0.14	4.16
C16:1/C18:1	0.13	0.37	0.58
C16:1/C18:2	0.19	0.54	0.94
C16:1/C18:3	1.11	1.90	0.86
C16:1/C20:0	0.26	2.07	27.30
C16:1/C22:0	6.32	0.76	14.56
C16:1/C22:1	-	3.95	15.67
C16:1/C24:0	-	3.09	2.07
C18:0/C18:1	0.43	2.57	0.14
C18:0/C18:2	0.63	3.71	0.23
C18:0/C18:3	3.65	13.09	0.21
C18:0/C20:0	0.85	14.30	6.57
C18:0/C22:0	20.83	5.25	3.50
C18:0/C22:1	-	27.30	3.77
C18:0/C24:0	-	21.34	0.50
C18:1/C18:2	1.44	1.46	1.61
C18:1/C18:3	5.19	5.10	1.48
C18:1/C20:0	5.60	5.57	46.77
C18:1/C22:0	48.33	2.04	24.95
C18:1/C22:1	-	10.63	26.84
C18:1/C24:0	-	8.31	3.55
C18:2/C18:3	5.76	3.53	0.91
C18:2/C20:0	1.34	3.85	29.00
C18:2/C22:0	1.43	1.41	15.47
C18:2/C22:1	-	7.36	16.64
C18:2/C24:0	-	5.75	2.20
C18:3/C20:0	0.23	0.40	31.71
C18:3/C22:0	5.71	0.40	16.91
C18:3/C22:1	-	2.09	18.20
C18:3/C24:0	-	1.63	2.41
C20:0/C22:0	24.46	0.37	0.53
C20:0/C22:1	-	1.91	0.57
C20:0/C24:0	-	1.49	0.08
C22:0/C22:1	-	5.20	1.08
C22:0/C24:0	-	4.06	0.14

C22:1/C24:0 - 0.78 0.13