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Acid-catalyzed algal biomass pretreatment for integrated lipid and carbohydrate-based biofuels production

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Electronic Supplementary Information (ESI)

Supplemental Table 1: Amino acid composition of representative algal biomass from 7 *Scenedesmus* sp. and 10 *Chlorella* sp. samples, with calculated nitrogen to protein conversion factors according to Mossé [32]. k_A = upper bound factor, k_P = lower bound factor, k = average conversion factor.

	Scenedesmus sp.							*Chlorella* sp.									
	early	early	mid	mid	late	late	late	early	early	early	mid	mid	mid	mid	late	late	late
%N	8.38	7.5	3.51	2.68	1.82	1.59	1.87	9.01	9.03	8	2.7	2.7	2.76	3.21	2.66	2.18	1.74
Weight % (AA):																	
L-Aspartic acid	3.73	3.11	1.56	0.78	0.70	0.65	0.69	3.87	3.63	3.19	1.13	1.15	1.17	1.40	0.91	0.93	0.74
L-Threonine	2.16	1.85	0.91	0.53	0.50	0.45	0.45	1.92	1.82	1.80	0.58	0.59	0.60	0.69	0.49	0.49	0.38
L-Serine	1.77	1.37	0.68	0.38	0.36	0.34	0.32	1.79	1.57	1.27	0.50	0.51	0.51	0.58	0.39	0.41	0.31
L-Glutamic Acid	4.34	3.27	1.80	0.80	0.74	0.73	0.72	4.96	4.98	3.63	1.33	1.38	1.29	1.68	0.96	1.04	1.13
L-Proline	1.93	1.72	0.84	0.46	0.44	0.39	0.39	1.93	1.98	2.12	0.59	0.61	0.63	0.73	0.48	0.48	0.40
L-Glycine	2.09	1.82	0.86	0.47	0.42	0.39	0.41	2.18	2.13	2.16	0.66	0.67	0.68	0.82	0.53	0.52	0.43
L-Alanine	3.21	2.76	1.39	0.76	0.69	0.67	0.66	3.45	3.19	3.48	1.23	1.26	1.21	1.25	1.02	1.07	0.71
L-Cysteine*	0.66	ND	ND	ND	0.20	0.18	ND	0.52	ND	ND	0.19	0.19	ND	ND	ND	0.18	ND
L-Valine	2.46	1.97	1.04	0.55	0.52	0.46	0.48	2.42	2.40	2.28	0.73	0.75	0.75	0.90	0.63	0.62	0.50
L-Methionine*	0.93	ND	ND	ND	0.24	0.19	ND	0.90	ND	ND	0.29	0.30	ND	ND	ND	0.23	ND
L-Isoleucine	1.72	1.37	0.73	0.37	0.36	0.32	0.32	1.70	1.60	1.58	0.49	0.50	0.50	0.62	0.40	0.40	0.32
L-Leucine	3.55	2.95	1.51	0.77	0.75	0.65	0.65	3.78	3.67	3.67	1.15	1.17	1.19	1.43	0.92	0.92	0.74
L-Tyrosine	1.39	1.15	0.60	0.31	0.28	0.26	0.27	1.66	1.60	1.41	0.51	0.52	0.50	0.63	0.39	0.41	0.33
L-Phenylalanine	2.24	1.93	0.97	0.50	0.49	0.42	0.42	2.52	2.17	2.35	0.73	0.74	0.74	0.92	0.56	0.59	0.45
L-Tryptophan	0.84	ND	ND	ND	0.17	0.15	ND	0.84	ND	ND	0.25	0.27	ND	ND	ND	0.17	ND
L-Lysine	2.38	1.76	0.92	0.40	0.38	0.39	0.38	2.64	3.65	1.80	0.74	0.75	0.72	0.88	0.58	0.60	0.49
L-Histidine	0.68	0.47	0.25	0.11	0.09	0.10	0.10	0.81	0.89	0.73	0.24	0.24	0.23	0.31	0.19	0.18	0.16
L-Arginine	2.39	1.80	0.90	0.44	0.40	0.43	0.38	2.78	2.78	2.02	0.76	0.77	0.76	0.91	0.58	0.63	0.48
k_A'	6.18	6.23	6.26	6.29	6.32	6.19	6.28	6.13	6.03	6.21	6.14	6.14	6.15	6.18	6.13	6.12	6.22
k_P	3.67	3.34	3.64	2.43	3.34	3.58	3.02	3.65	3.61	3.58	3.60	3.68	3.55	3.67	2.90	3.64	3.72
k	4.93	4.79	4.95	4.36	4.83	4.89	4.65	4.89	4.82	4.89	4.87	4.91	4.85	4.92	4.52	4.88	4.97

Supplemental Table 2: Key modeling inputs and yields for TEA evaluation of fractionation process mid-harvest *Scenedesmus* sp. case; experimental fractionation baseline and improved process scenarios. RD = Renewable diesel, AD = Anaerobic digestion

Metric	Baseline assumption	Improved assumption
Sugar yield in pretreatment (*% theoretical and g/g biomass*)	65% = 0.30 g/g	90% = 0.42 g/g
Pretreatment acid loading (*based on feed liquor weight*)	2%	1%
Sugar conversion to ethanol *(% and g ethanol/g sugar*)[1]	82% = 0.42 g/g	95% = 0.48 g/g
Net overall lipid extraction efficiency	86%	90%
RD yield per mass algae feed	16.9 wt% = 55.4 GGE/ton	17.8 wt% = 58.5 GGE/ton
Ethanol yield per mass algae feed	7.5 wt% = 15.0 GGE/ton	13.5 wt% = 27.0 GGE/ton
AD operating conditions	20 day retention time, 35 °C temperature	
AD carbon destruction to biogas	48%	
Biogas methane yield from feed solids	0.29 L CH_4/g TS, baseline vs improved cases[2]	
AD nutrient recovery in effluent	80% N, 50% P; 5% loss of N (as NH_3) during recycle	

[1] Metabolic yield from sugars available for fermentation; does not include sugar diversion to seed train (10%) or assumed contamination losses (3%) built into model. Also does not include upstream sugar losses from solid-liquid separation (centrifugation).

[2] All cases assume AD biogas composition = 67 vol% CH_4, 33 vol% CO_2 [5]