Electronic Supplementary Information (ESI)

Production of Platform Molecules from Sweet Sorghum

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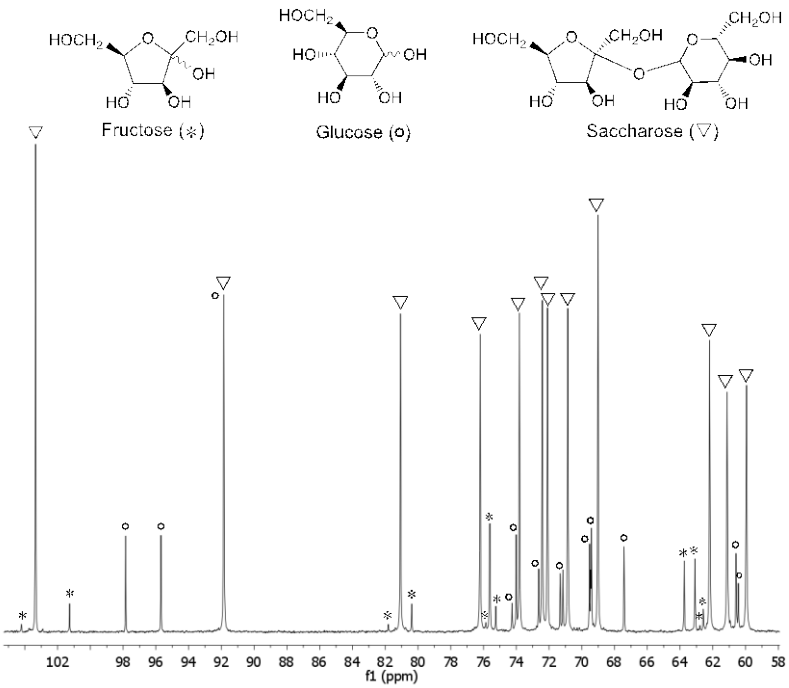
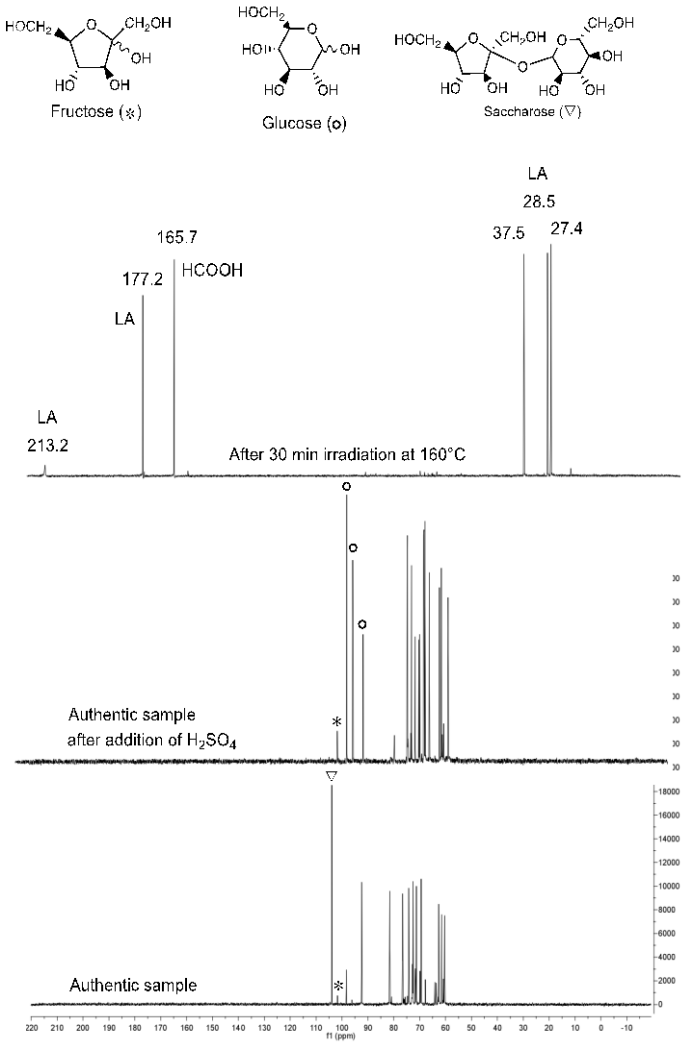
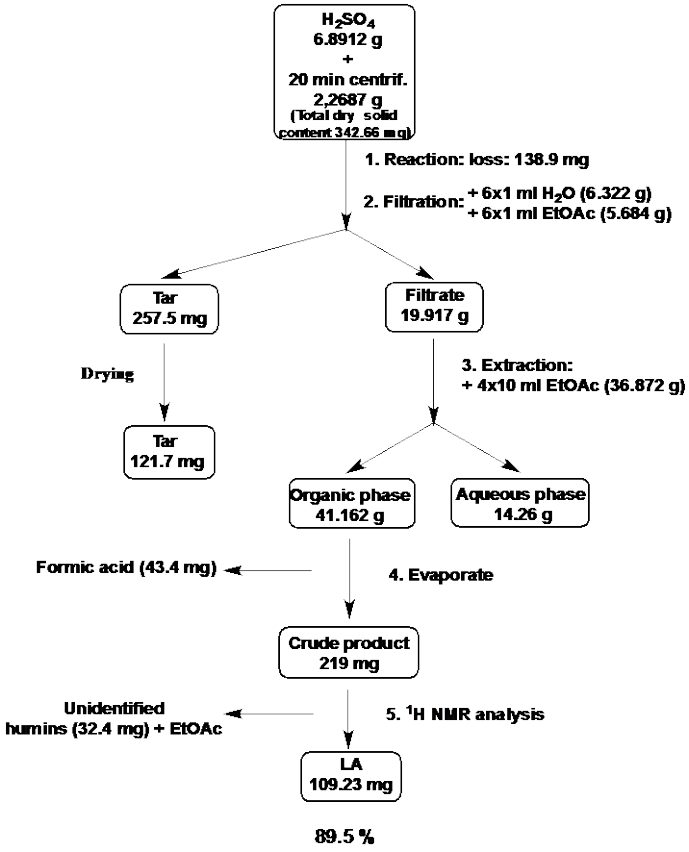


ESI-Fig. S1. ^{13}C-NMR spectrum of sweet sorghum juice.



ESI-Fig. S2. ^{13}C-NMR spectrum of sweet sorghum juice.



ESI-Fig. S3. Mass balance of the process

NMR Calculations

The yield ($m_{\text{levulinic acid}}/m_{\text{total dry mass of the sweet sorghum sample}}$) of levulinic acid was calculated from the ^{1}H-NMR spectrum using benzene (10 µL, m = 8.786 mg, n = 0.113 mmol) as an internal standard. The formula used to calculate the amount of levulinic acid:

$$n_{LA} = \frac{2 \cdot n_B \cdot I_{LA}}{I_B} = 2 \cdot n_B \cdot I_{LA} = 0.000226 \cdot I_{LA} \qquad \text{(Eq. 1.)}$$

where: n_B = mol of benzene added, n_{LA} = mol of levulinic acid formed, I_B = ^{1}H-NMR integral of benzene (6H) was set to 1., I_{LA} = ^{1}H-NMR integral of peak of levulinic acid at 2.1 ppm (-CH_3; 3H).

ESI – Table S1. Conversion of crude sweet sorghum juice to levulinic acid

Entry	Time (min)	Temp (°C)	TDS content (g/L)	Integral (I_{LA})	LA (mg)	Yield (wt%)
1	15	100	197	0.02	0.64	0.16
2	15	120	197	0.62	16.22	4.12
3	15	140	197	1.33	34.84	8.84
4	15	160	197	1.46	38.15	9.68
5	15	180	197	0.84	21.93	5.57
6	15	200	197	0.62	16.24	4.12
7	30	100	197	0.10	2.51	0.64
8	30	120	197	0.73	19.08	4.84
9	30	140	197	1.72	44.79	11.37
10	30	160	197	2.29	59.71	15.15
11	30	180	197	1.91	49.83	12.64
12	30	200	197	1.19	30.97	7.86
13	45	100	197	0.16	4.12	1.05
14	45	120	197	0.87	22.78	5.78
15	45	140	197	1.58	41.26	10.47
16	45	160	197	1.87	48.96	12.43
17	45	180	197	1.41	36.72	9.32
18	45	200	197	1.04	27.07	6.87

ESI – Table S2. Conversion of pretreated (20 min centrifugation) sweet sorghum juice to levulinic acid

Entry	Time (min)	Temp (°C)	TDS content (g/L)	Integral (I_{LA})	LA (mg)	Yield (wt%)
1	15	100	171	0.15	3.84	1.12
2	15	120	171	0.72	18.93	5.52
3	15	140	171	1.44	37.51	10.95
4	15	160	171	3.13	81.73	23.85
5	15	180	171	2.85	74.32	21.69
6	15	200	171	2.08	54.22	15.82
7	30	100	171	0.50	13.00	3.79
8	30	120	171	1.32	34.45	10.06
9	30	140	171	1.97	51.46	15.02
10	30	160	171	4.12	107.61	31.40
11	30	180	171	3.35	87.59	25.56
12	30	200	171	2.32	60.65	17.70
13	45	100	171	0.71	18.67	5.45
14	45	120	171	1.47	38.29	11.18
15	45	140	171	2.20	57.57	16.80
16	45	160	171	3.78	98.74	28.82
17	45	180	171	3.21	83.82	24.46
18	45	200	171	2.45	64.11	18.71

ESI – Table S3. Conversion of pretreated (40 min centrifugation) sweet sorghum juice to levulinic acid

Entry	Time (min)	Temp (°C)	TDS content (g/L)	Integral (I_{LA})	LA (mg)	Yield (wt%)
1	15	100	186	0.16	4.10	1.10
2	15	120	186	0.54	14.21	3.81
3	15	140	186	1.30	34.03	9.13
4	15	160	186	1.70	44.45	11.93
5	15	180	186	1.29	33.59	9.02
6	15	200	186	0.86	22.54	6.05
7	30	100	186	0.23	6.11	1.64
8	30	120	186	1.13	29.44	7.90
9	30	140	186	1.87	48.96	13.14
10	30	160	186	2.49	65.00	17.44
11	30	180	186	1.62	42.21	11.33
12	30	200	186	1.24	32.39	8.69
13	45	100	186	0.34	8.81	2.36
14	45	120	186	0.95	24.78	6.65
15	45	140	186	1.57	40.98	11.00
16	45	160	186	2.00	52.13	13.99
17	45	180	186	1.34	34.89	9.36
18	45	200	186	1.03	26.81	7.20

ESI – Table S4. Conversion of pretreated (60 min centrifugation) sweet sorghum juice to levulinic acid

Entry	Time (min)	Temp (°C)	TDS content (g/L)	Integral (I_{LA})	LA (mg)	Yield (wt%)
1	15	100	196	0.03	0.70	0.18
2	15	120	196	0.65	17.03	4.33
3	15	140	196	1.42	37.13	9.44
4	15	160	196	1.65	43.12	10.97
5	15	180	196	1.12	29.31	7.45
6	15	200	196	1.09	28.49	7.25
7	30	100	196	0.10	2.62	0.67
8	30	120	196	0.80	20.81	5.29
9	30	140	196	2.18	56.92	14.48
10	30	160	196	2.65	69.20	17.60
11	30	180	196	1.84	48.18	12.25
12	30	200	196	1.33	34.81	8.85
13	45	100	196	0.28	7.24	1.84
14	45	120	196	0.99	25.73	6.54
15	45	140	196	1.93	50.39	12.81
16	45	160	196	2.14	55.95	14.23
17	45	180	196	1.77	46.31	11.78
18	45	200	196	1.18	30.91	7.86

ESI – Table S5. Conversion of pretreated (90 min centrifugation) sweet sorghum juice to levulinic acid

Entry	Time (min)	Temp (°C)	TDS content (g/L)	Integral (I_{LA})	LA (mg)	Yield (wt%)
1	15	100	202	0.03	0.74	0.19
2	15	120	202	0.63	16.47	4.14
3	15	140	202	1.17	30.62	7.69
4	15	160	202	1.40	36.62	9.19
5	15	180	202	1.24	32.51	8.16
6	15	200	202	0.97	25.39	6.37
7	30	100	202	0.14	3.63	0.91
8	30	120	202	1.15	29.92	7.51
9	30	140	202	1.94	50.74	12.74
10	30	160	202	2.38	62.19	15.61
11	30	180	202	1.68	43.85	11.01
12	30	200	202	1.28	33.39	8.38
13	45	100	202	0.20	5.15	1.29
14	45	120	202	1.01	26.50	6.65
15	45	140	202	1.65	43.06	10.81
16	45	160	202	2.04	53.39	13.40
17	45	180	202	1.41	36.77	9.23
18	45	200	202	1.08	28.08	7.05

Calculation of settling regions[1]

ρ_p: density of particles (wet starch density, kg/m^3)

ρ_f: density of sweet sorghum juice (kg/m^3)

η_f: dynamic viscosity of sweet sorghum juice (Pa·s)

l: height of bowl of centrifuge (m)

t: time required to settle in gravity field (s, min, h, day)

d: diameter of particles (μm)

g: acceleration of gravity (m/s^2)

u: velocity of the particles (m/s)

B: defined as:

$$B = \sqrt[3]{\frac{4}{3} \cdot \frac{(\rho_p - \rho_f) \cdot \rho_f \cdot g}{\eta_f^2}}$$

F(d) dimensionless number defines as:

$$F(d) = B \cdot d_p$$

[1] (a) J. Hunek and J. Sawinsky, Chemical Engineering, National Academic Press, Budapest, 1983. (b) Perry's Chemical Engineers' Handbook, 8th ed., McGraw-Hill Education, 2007; (c) Coulson and Richardson's Chemical Engineering, 5th ed. Vol. 2 (Particle Technology and Separation Processes), Butterworth-Heinemann, Oxford, 2002.

F(u) dimensionless number in the Stokes-region defines as:

$$F(u)=\frac{F(d)^2}{24} \quad \text{and:} \quad F(u)=\frac{u\cdot\rho_f}{B\cdot\eta_f}$$

ESI – Table S6. Calculation of time required to settle in gravity field

	Entry 1	Entry 2	Entry 3	Entry 4	Entry 5	Entry 6
ρ_p (kg/m^3)	1305	1305	1305	1305	1315	1315
d (μm)	0.1	0.8	3	300	0.1	300
ρ_f (kg/m^3)	1082.8	1082.8	1082.8	1082.8	1082.8	1082.8
η_f (Pa·s)	0.00176	0.00176	0.00176	0.00176	0.00176	0.00176
d (m)	10^{-7}	$8\cdot10^{-7}$	$3\cdot10^{-6}$	$3\cdot10^{-4}$	10^{-7}	$3\cdot10^{-4}$
B	10052.905	10052.905	10052.905	10052.905	10201.506	10201.506
F(d)	$1.005\cdot10^{-3}$	$8.042\cdot10^{-3}$	$3.016\cdot10^{-2}$	3.016	$1.020\cdot10^{-3}$	3.060
Stokes-range?	Stokes	Stokes	Stokes		Stokes	
Transient range?				transient		transient
F(u) calculated	$4.211\cdot10^{-8}$	$2.695\cdot10^{-6}$	$3.790\cdot10^{-5}$		$4.336\cdot10^{-8}$	
F(u) from graph				0.3		0.3
u (m/s)	$6.881\cdot10^{-10}$	$4.404\cdot10^{-8}$	$6.193\cdot10^{-7}$	$4.902\cdot10^{-3}$	$7.190\cdot10^{-10}$	$4.975\cdot10^{-3}$
l (m)	0.09	0.09	0.09	0.09	0.09	0.09
t (s)	$1.308\cdot10^{8}$	$2.044\cdot10^{6}$	$1.453\cdot10^{5}$	$1.836\cdot10^{1}$	$1.252\cdot10^{8}$	$1.809\cdot10^{1}$
t (min)	$2.180\cdot10^{6}$	$3.406\cdot10^{4}$	$2.422\cdot10^{3}$	$3.060\cdot10^{-1}$	$2.086\cdot10^{6}$	$3.015\cdot10^{-1}$
t (h)	$3.633\cdot10^{4}$	$5.677\cdot10^{2}$	40.370	$5.100\cdot10^{-3}$	$3.477\cdot10^{4}$	$5.026\cdot10^{-3}$
t (day)	$1.514\cdot10^{3}$	23.65	1.682	$2.125\cdot10^{-4}$	$1.449\cdot10^{3}$	$2.094\cdot10^{-4}$
Conclusion	too much time centrifugation required	too much time centrifugation required	too much time centrifugation required	too much time centrifugation required	too much time centrifugation required	too much time centrifugation required

Detailed calculation for Entry 1:

$$B=\sqrt[3]{\frac{4}{3}\cdot\frac{\left(1305\frac{kg}{m^3}-1082.8\frac{kg}{m^3}\right)\cdot1082.8\frac{kg}{m^3}\cdot9.81\frac{m}{s^2}}{0.00176^2(Pa\cdot s)^2}}=10052.905\frac{1}{m}$$

$$F(d)=10052.905\frac{1}{m}\cdot10^{-7}m=1.005\cdot10^{-3}$$

$$F(u)=\frac{\left(1.005\cdot10^{-3}\right)^2}{24}=4.211\cdot10^{-8}$$

$$u = \frac{4.211 \cdot 10^{-8} \cdot 10052.905 \frac{1}{m} \cdot 0.00176 Pa \cdot s}{1082.8 \frac{kg}{m^3}} = 6.88 \cdot 10^{-10} \frac{m}{s}$$

Time required to settle in gravity field, taking into account the sedimentation length i.e. the height of bowl (0.09m)

$$t = \frac{0.09 m}{8.88 \cdot 10^{10} \frac{m}{s}} = 1.308 \cdot 10^{8} s$$