SUPPORTING INFORMATION

MgO/CaO nanocomposite facilitates economical production of D-fructose and D-allulose using glucose and its response prediction using a DNN model

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Mathematical expressions:

$$Glucose\ conversion\ (wt.\%) = \frac{(Intial\ wt.of\ glucose - Remaining\ wt.of\ glucose\ after\ completion\ of\ reaction)}{Intial\ wt.of\ glucose}$$

------- (S1)

$$Product\ yield\ (wt.\%) = \frac{Wt.of\ product\ formation}{Initial\ wt.of\ glucose} \times 100$$

------- (S2)

$$Product\ selectivity\ (wt.\%) = \frac{Wt.of\ product\ formation}{Converted\ wt.of\ glucose} \times 100$$

------- (S3)

Second-order polynomial equation:

$$y = a_0 + \sum_{i=1}^{k} a_i X_i + \sum_{i=1}^{k} a_{ij} X_j^2 + \sum_{i<j}^{k} \sum_{j}^{k} a_{ij} X_i X_j + e \quad \text{for } i<j$$ ------- (S4)

Where, a_0 is a constant; *i* and *j* are the linear and quadratic coefficients; *a* is the regression coefficient; *k* is the number of factors investigated in the experimental trials; *e* is the random error.

Debye-Scherrer's equation:

$$D = \frac{K \times \lambda}{\beta \times Cos\theta}$$ ------- (S5)

where *K* is the constant; λ is the incident wavelength of X-ray (1.54056 Å); β is full width at half maxima (FWHM); and *θ* is the Bragg's angle and the values are listed in the below Table S1.

Interplanar spacing calculation (d-spacing):

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

------- (S6)

Where, d_{hkl} is the spacing between the adjacent planes, *h*, *k*, and *l* are the miller indices of (200) plane and *a* is the lattice parameter of a cubic lattice with allowed reflections.

Kinetic rate constant calculation:

Irreversible reaction(s)

$$Glucose \xrightarrow{rate\ constant,\ k} Fructose$$ ------- (S7)

Rate equation(s)

$$ln\left\{\frac{[Glu]_t}{[Glu]_0}\right\} = -k \times time \text{ (sec)}$$ ------- (S8)

Where, $[Glu]_t$ and $[Glu]_0$ represent the final and initial glucose concentrations at time *t*. *k* is the first-order rate constant of disappearance of glucose.

Table S1. Result of BET analysis on the as-synthesized catalysts.

S. No	Catalyst	Molar ratio of Ca/Mg[a]	Surface area[b] (m^2/g)	Pore volume[b] (cc/g)	Average pore Diameter[b] (10^2 Å)
1	MgO	0.0/1.0	37.269	0.386	2.1
2	CaO	1.0/0.0	20.868	0.136	1.3
3	CM-A	1.0/0.42	20.069	0.096	1.0
4	CM-B	1.0/1.01	30.311	0.251	1.7
5	CM-C	1.0/2.03	31.899	0.389	2.6

[a] Values obtained from ICP measurements. [b] Values calculated from N_2 adsorption isotherms (BET method).

Table S2. *d*-spacing and crystallite size of the nanocomposites estimated from the XRD results.

Sample	(hkl) plane	2θ (degree)	FWHM (degree)	d-spacing (d_{hkl}) (Å)	Crystallite size (nm)
MgO	(200)	42.88	0.34676	2.1083	25.70
CaO	(200)	37.39	0.14489	2.3987	60.43
Mg:Ca 1:1 (MC-A)	(200)	37.39	0.25256	2.4036	34.67
Mg:Ca 1:2 (MC-B)	(200)	37.39	0.21457	2.3948	40.81
Mg:Ca 2:1 (MC-C)	(200)	37.39	0.31535	2.4012	27.77

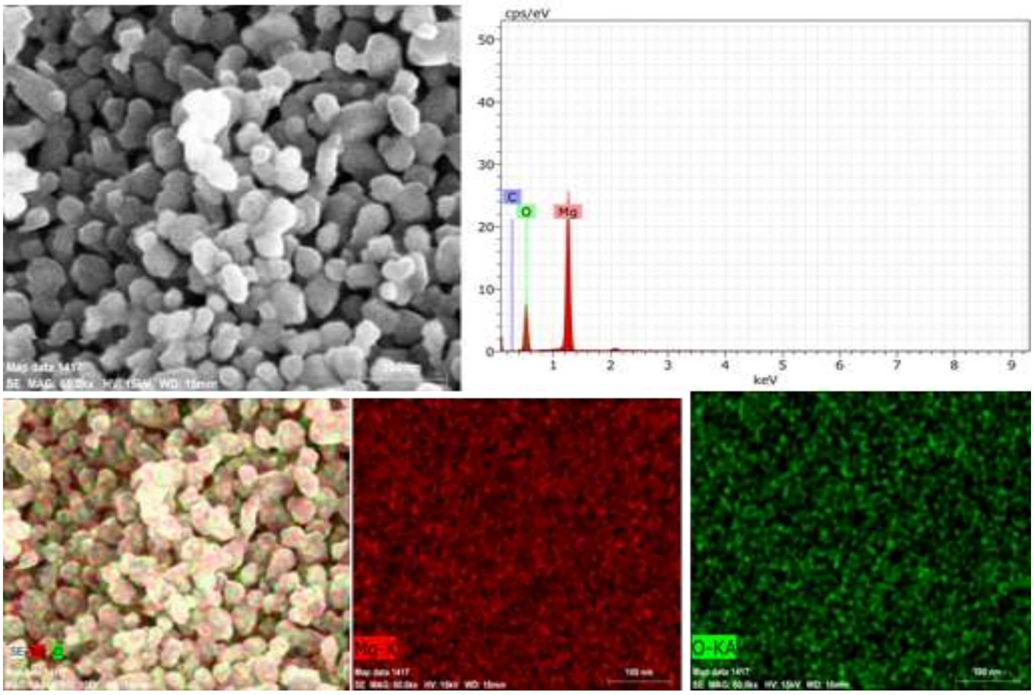

Fig. S1. FE-SEM-EDX and elemental mapping of synthesised pristine MgO catalyst.

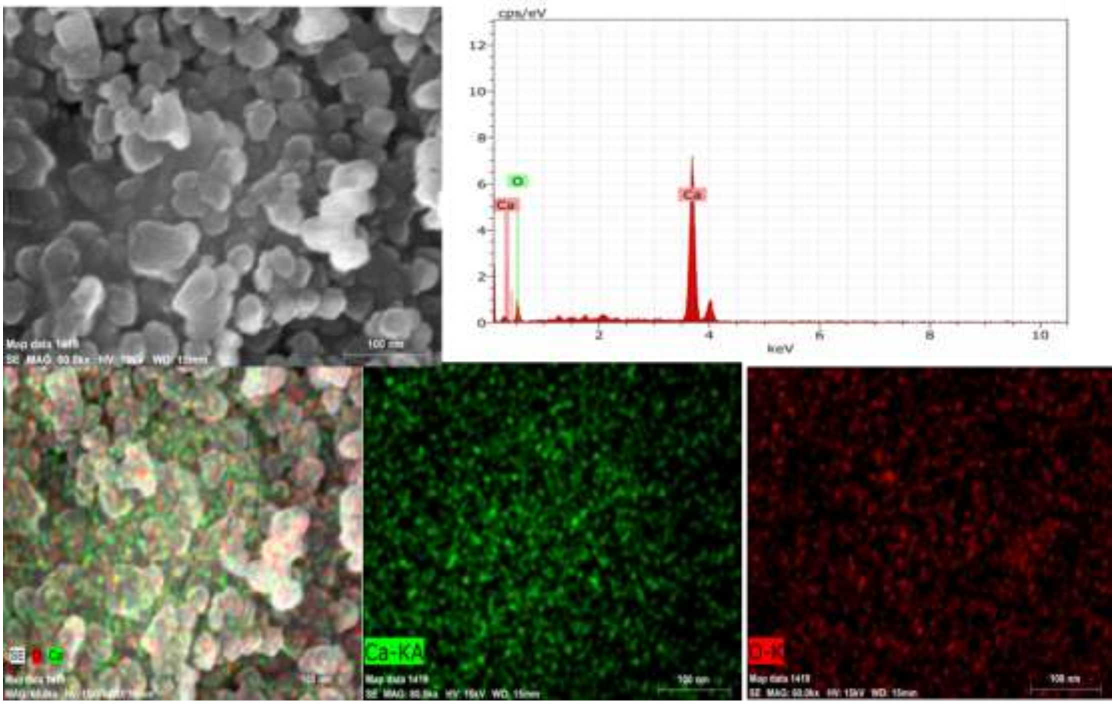

Fig. S2. FE-SEM-EDX and elemental mapping of synthesised pristine CaO catalyst.

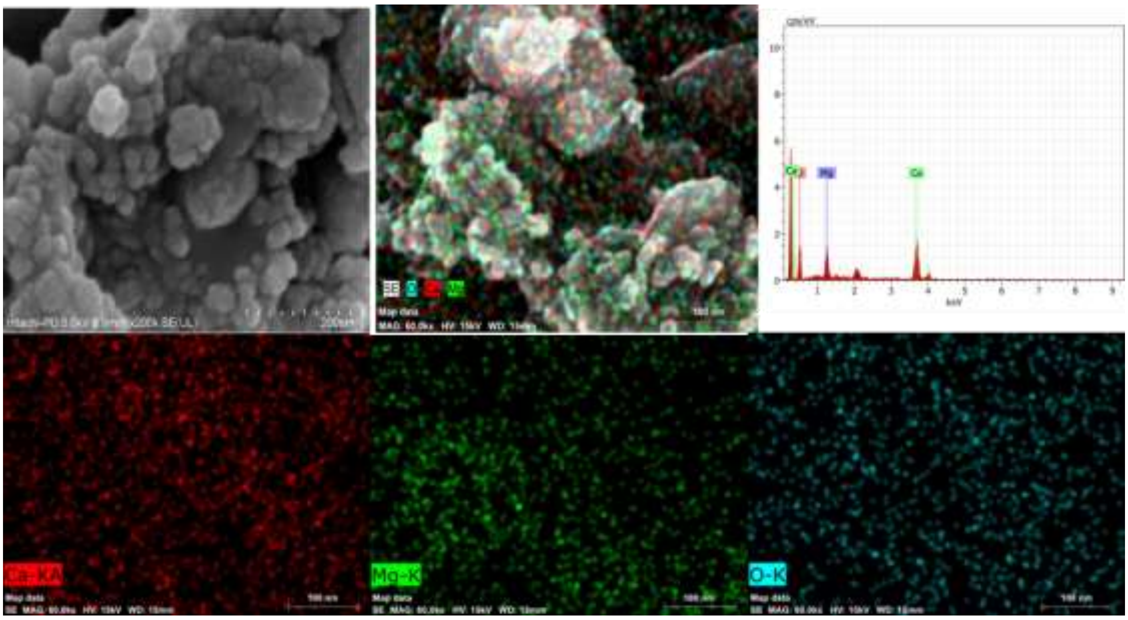

Fig. S3. FE-SEM-EDX and elemental mapping of synthesised MC-A composite.

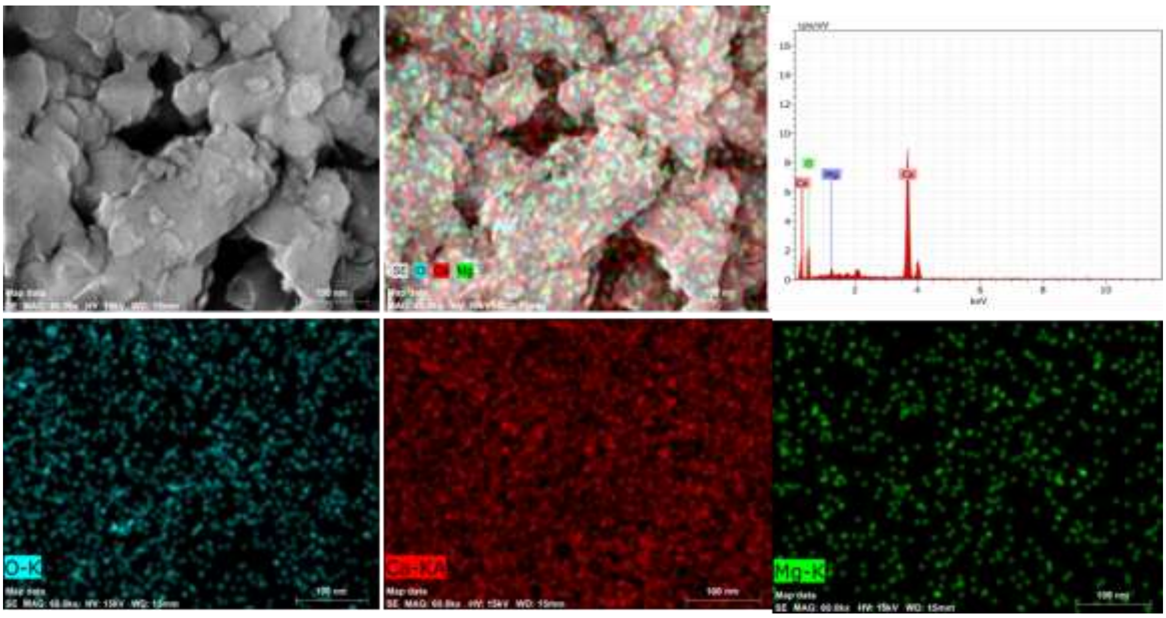

Fig. S4. FE-SEM-EDX and elemental mapping of synthesised MC-B composite.

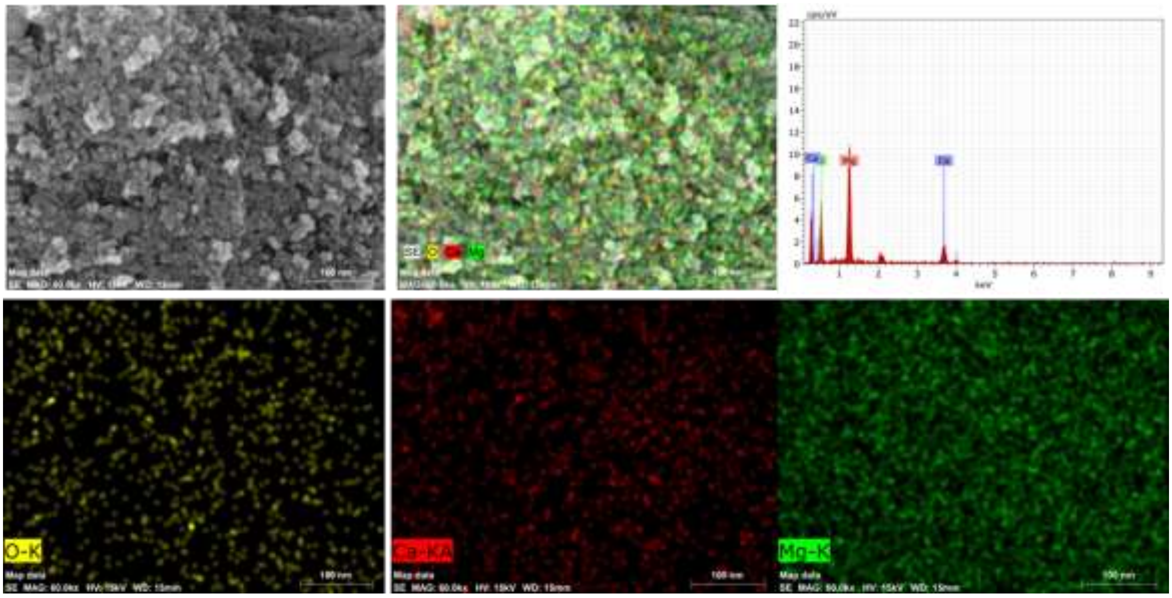

Fig. S5. FE-SEM-EDX and elemental mapping of synthesised MC-C composite.

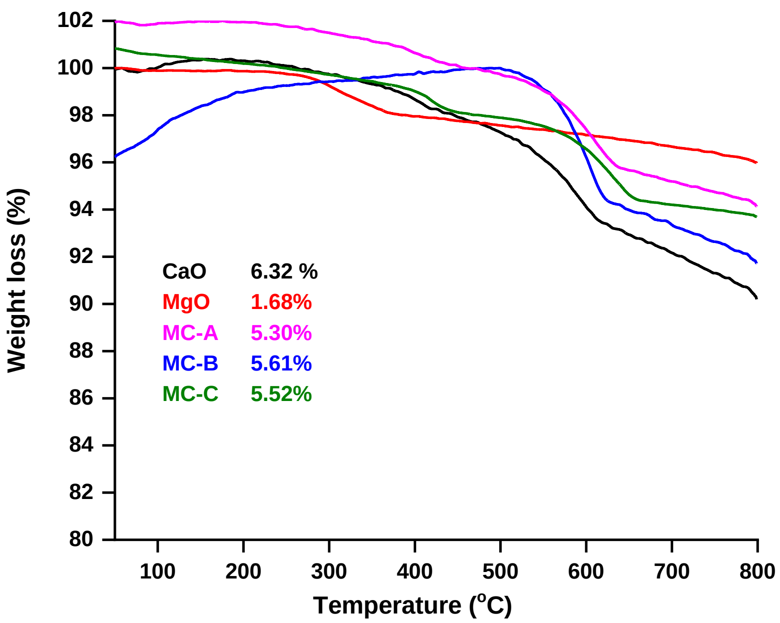

Fig. S6. TGA curves of the corresponding as-synthesised catalysts measured in the temperature range from 50 °C to 800 °C.

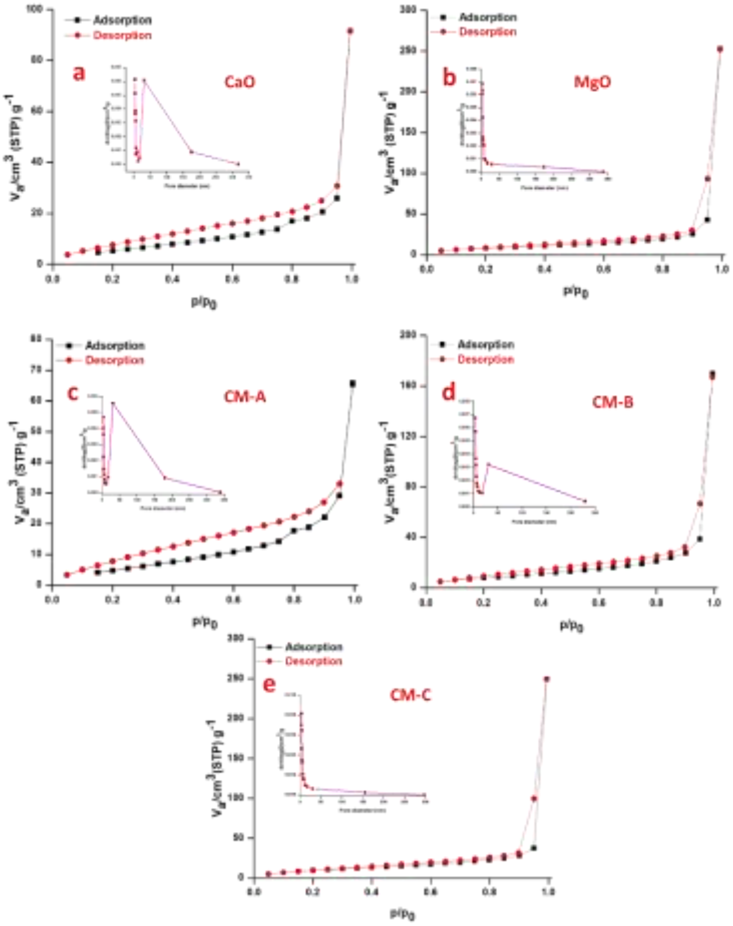

Fig. S7. N_2-physisorption isotherm of the as-synthesized pristine CaO (a), pristine MgO (b), CM-A (c), CM-B (d) and CM-C (e). Inset: BJH distribution curve.

Table S3. Acidic and basic properties of synthesized catalysts by CO_2/NH_3-TPD analysis

S.No	Catalyst	Basic sites (µmol CO_2/g)				Total Acidic sites (µmol NH_3/g)
		Weak	Moderate	Strong	Total	
1	MgO	157.0	45.0	--	202.0	38.0
2	CaO	17.0	87.0	323.0	427.0	28.0
3	MC-A	12.0	47.0	244.0	303.0	33.0
4	MC-B	11.0	22.0	225.0	258.0	37.0
5	MC-C	17.0	41.0	254.0	312.0	30.0

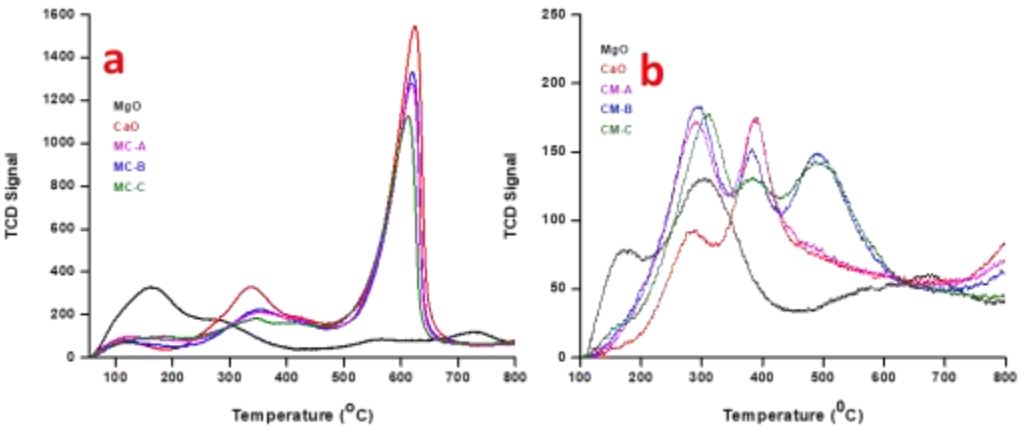

Fig. S8. TPD profile of the as-synthesized pristine CaO and MgO and their composites (CM-A, CM-B and CM-C). (a) CO_2 absorption profile and (b) NH_3 absorption profile.

Table S4. Catalytic activity of synthesised catalysts in the isomerization of glucose[a]

S.No	Sample Code	Glucose Conversion (%)	Fructose yield (%)	Mannose yield (%)	Psicose yield (%)	Fructose selectivity (%)	Carbon Balance (%)
1	CaO	59.0	27.0	6.1	6.2	45.7	66.61
2	MgO	33.5	24.9	4.0	4.6	74.3	100.00
3	MC-A	41.2	33.0	3.4	2.7	80.0	94.90
4	MC-B	58.0	28.7	4.4	3.1	49.4	62.41
5	MC-C	56.5	30.9	6.1	4.2	54.6	72.92

[a]Reaction conditions: 100 mg glucose, 3.0 mg catalyst, 5.0 mL water, 120 °C temperature, 15 min, 3.0 mg catalyst.

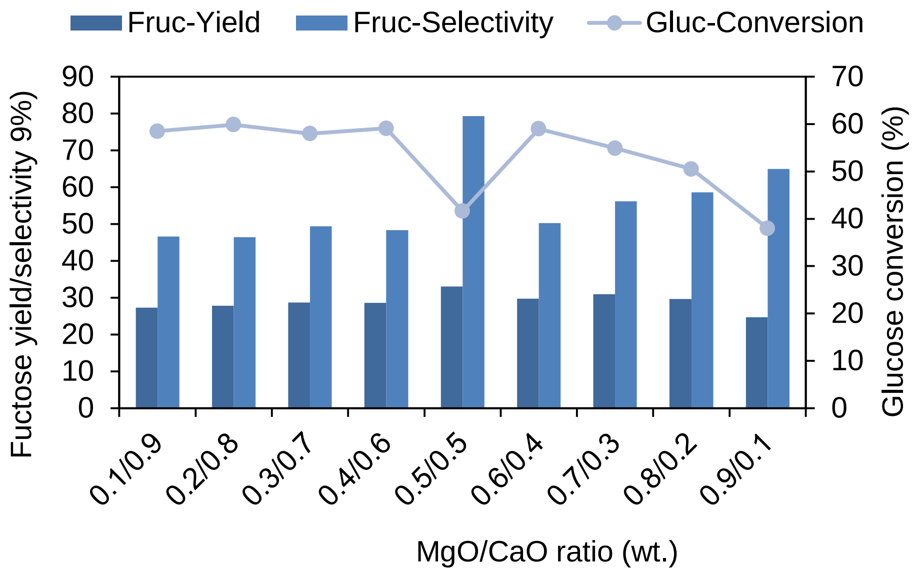

Fig. S9. Effect of MgO/CaO ratio on fructose synthesis in an aqueous condition (at 120 °C for 15 min using 3% catalyst loading).

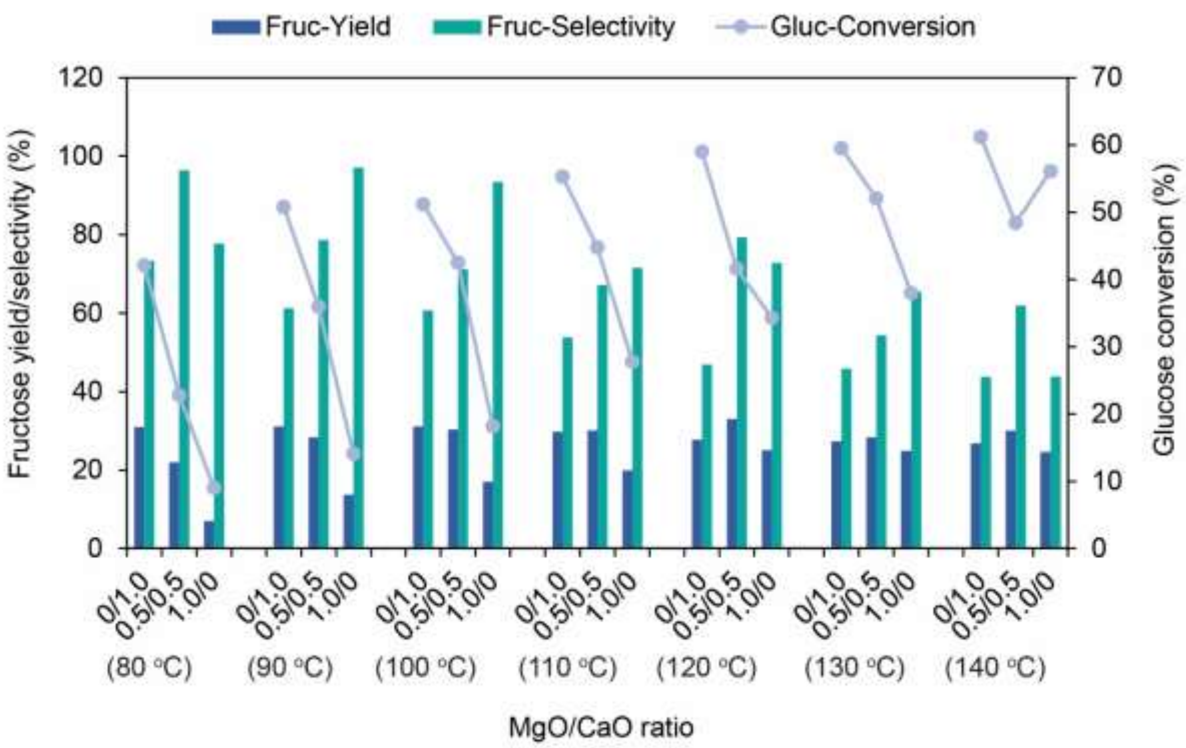

Fig. S10. Effect of temperature on fructose formation in an aqueous condition (at 3% catalyst loading for 15 min) using pristine and nanocomposite materials (MgO/CaO).

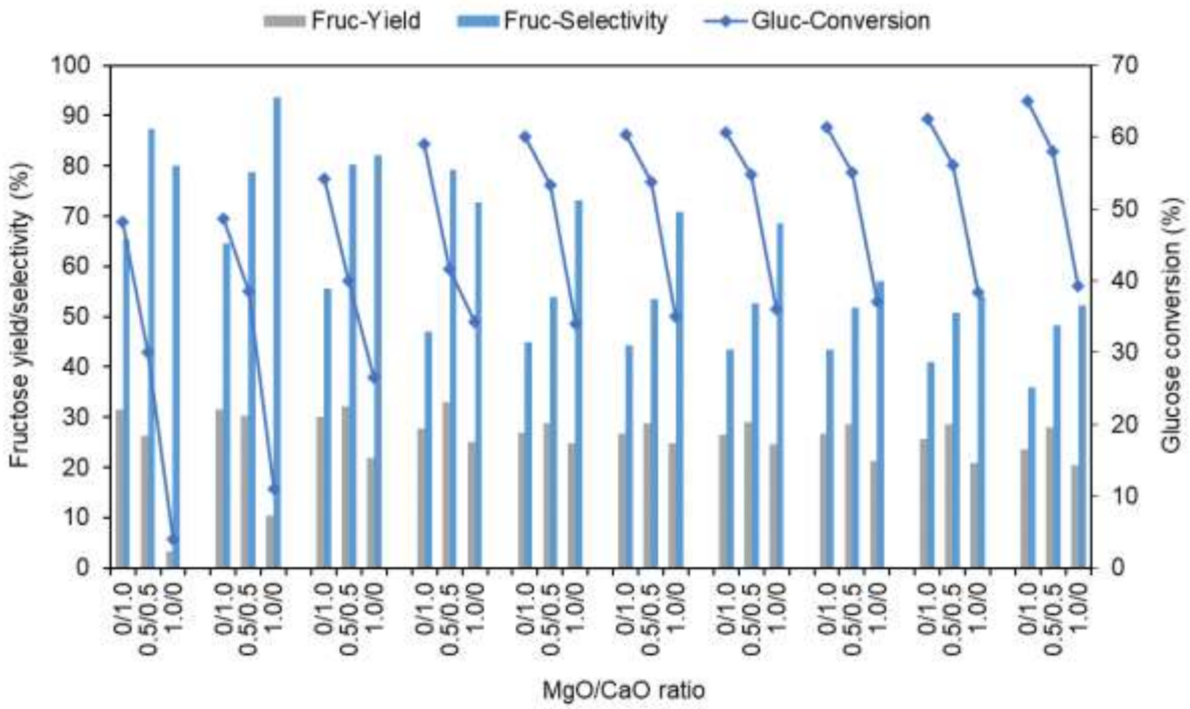

Fig. S11. Effect of time on fructose formation in an aqueous condition (at 120 °C and 3% catalyst loading) using pristine and nanocomposite materials (MgO/CaO).

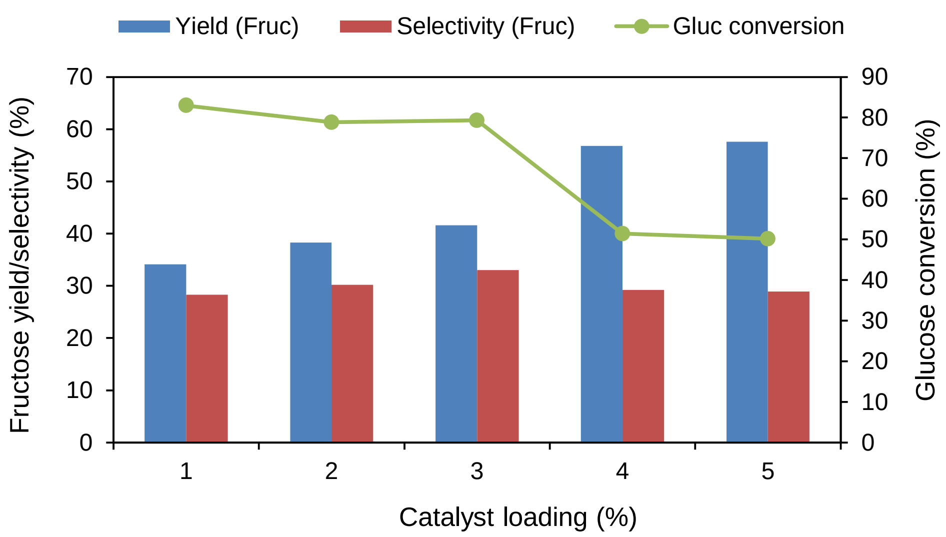

Fig. S12. Effect of catalyst loading under optimum conditions (120 °C for 15 min) using MC-A.

Table S5. Data obtained from various molar ratio combinations of the MgO and CaO in nano-composites used for machine learning studies.

Runs	Molar ratio of MgO	Molar ratio of CaO	Time (min.)	Temperature (^{o}C)	Yield of Fructose (%)	Conversion of Glucose (%)	Selectivity of Fructose (%)
1	0	1	3	120	31.5	48.2	65.3
2	0.1	0.9	3	120	30.8	49.4	62.3
3	0.2	0.8	3	120	29.7	50.0	59.4
4	0.3	0.7	3	120	30.0	42.0	71.4
5	0.4	0.6	3	120	24.2	46.7	51.8
6	0.5	0.5	3	120	26.3	30.1	87.3
7	0.6	0.4	3	120	23.5	29.0	81.0
8	0.7	0.3	3	120	26.2	37.7	69.4
9	0.8	0.2	3	120	13.1	18.9	69.3
10	0.9	0.1	3	120	5.6	6.7	83.5
11	1	0	3	120	3.2	4.0	80.0
12	0	1	5	120	31.5	48.7	64.6
13	0.1	0.9	5	120	30.9	48.6	63.5
14	0.2	0.8	5	120	28.4	59.3	47.8
15	0.3	0.7	5	120	31.0	46.2	67.0
16	0.4	0.6	5	120	25.0	57.1	43.7
17	0.5	0.5	5	120	30.3	38.5	78.7
18	0.6	0.4	5	120	26.8	55.5	48.2
19	0.7	0.3	5	120	30.7	48.4	63.4
20	0.8	0.2	5	120	26.3	33.1	79.4
21	0.9	0.1	5	120	18.6	23.0	80.8
22	1	0	5	120	10.3	11.0	93.6
23	0	1	10	120	30.1	54.2	55.5
24	0.1	0.9	10	120	29.9	54.0	55.3
25	0.2	0.8	10	120	28.1	58.8	47.7
26	0.3	0.7	10	120	28.8	57.0	50.5
27	0.4	0.6	10	120	25.5	58.3	43.7
28	0.5	0.5	10	120	32.1	40.0	80.2
29	0.6	0.4	10	120	28.6	58.0	49.3
30	0.7	0.3	10	120	30.3	55.5	54.5
31	0.8	0.2	10	120	29.7	49.3	60.2
32	0.9	0.1	10	120	24.5	34.1	71.8
33	1	0	10	120	21.8	26.5	82.2
34	0	1	15	120	27.7	59.0	46.9
35	0.1	0.9	15	120	27.3	58.5	46.6
36	0.2	0.8	15	120	27.8	59.9	46.4
37	0.3	0.7	15	120	28.7	58.0	49.4
38	0.4	0.6	15	120	28.6	59.1	48.3
39	0.5	0.5	15	120	33.0	41.6	79.3
40	0.6	0.4	15	120	29.7	59.0	50.3
41	0.7	0.3	15	120	30.9	54.9	56.2
42	0.8	0.2	15	120	29.6	50.5	58.6
43	0.9	0.1	15	120	24.7	38.0	65.0
44	1	0	15	120	25.0	34.3	72.8
45	0	1	20	120	27.0	60.1	44.9
46	0.1	0.9	20	120	26.5	60.3	43.9
47	0.2	0.8	20	120	27.4	61.2	44.7
48	0.3	0.7	20	120	28.8	58.2	49.4
49	0.4	0.6	20	120	29.8	60.1	49.5

50	0.5	0.5	20	120	28.8	53.3	54.0
51	0.6	0.4	20	120	30.3	56.3	53.8
52	0.7	0.3	20	120	28.0	59.7	46.9
53	0.8	0.2	20	120	29.8	54.5	54.6
54	0.9	0.1	20	120	24.7	35.2	70.1
55	1	0	20	120	24.9	34.0	73.2
56	0	1	25	120	26.7	60.4	44.2
57	0.1	0.9	25	120	25.9	61.2	42.3
58	0.2	0.8	25	120	27.1	62.3	43.4
59	0.3	0.7	25	120	28.6	58.5	48.8
60	0.4	0.6	25	120	27.5	61.6	44.6
61	0.5	0.5	25	120	28.8	53.8	53.5
62	0.6	0.4	25	120	28.9	63.2	45.7
63	0.7	0.3	25	120	28.1	59.2	47.4
64	0.8	0.2	25	120	28.7	57.7	49.7
65	0.9	0.1	25	120	24.4	37.6	64.8
66	1	0	25	120	24.8	35.0	70.8
67	0	1	30	120	26.4	60.6	43.5
68	0.1	0.9	30	120	26.8	62.2	43.0
69	0.2	0.8	30	120	27.0	63.0	42.8
70	0.3	0.7	30	120	28.2	58.8	47.9
71	0.4	0.6	30	120	27.6	61.6	44.8
72	0.5	0.5	30	120	28.9	54.8	52.7
73	0.6	0.4	30	120	28.4	61.4	46.2
74	0.7	0.3	30	120	27.5	61.9	44.4
75	0.8	0.2	30	120	28.4	58.3	48.7
76	0.9	0.1	30	120	26.1	44.7	58.3
77	1	0	30	120	24.7	36.0	68.6
78	0	1	40	120	26.7	61.4	43.4
79	0.1	0.9	40	120	26.2	61.1	58.3
80	0.2	0.8	40	120	26.3	62.6	42.0
81	0.3	0.7	40	120	28.1	58.8	47.5
82	0.4	0.6	40	120	27.6	65.4	42.2
83	0.5	0.5	40	120	28.6	55.1	51.9
84	0.6	0.4	40	120	28.0	62.3	44.9
85	0.7	0.3	40	120	27.6	62.0	44.5
86	0.8	0.2	40	120	28.7	59.4	48.3
87	0.9	0.1	40	120	21.7	47.8	45.3
88	1	0	40	120	21.2	37.1	57.1
89	0	1	50	120	25.7	62.6	41.0
90	0.1	0.9	50	120	25.7	62.1	41.3
91	0.2	0.8	50	120	25.6	64.7	39.5
92	0.3	0.7	50	120	27.7	59.1	46.8
93	0.4	0.6	50	120	26.5	65.4	40.5
94	0.5	0.5	50	120	28.5	56.1	50.8
95	0.6	0.4	50	120	27.8	62.4	44.5
96	0.7	0.3	50	120	27.5	62.2	44.2
97	0.8	0.2	50	120	27.5	60.5	45.4
98	0.9	0.1	50	120	20.7	40.2	51.4
99	1	0	50	120	20.8	38.4	54.1
100	0	1	60	120	23.5	65.1	36.0
101	0.1	0.9	60	120	23.9	64.8	36.8
102	0.2	0.8	60	120	25.7	64.7	39.7
103	0.3	0.7	60	120	27.5	59.7	46.0
104	0.4	0.6	60	120	26.5	66.3	39.9
105	0.5	0.5	60	120	28.0	58.0	48.2
106	0.6	0.4	60	120	27.6	64.1	43.0
107	0.7	0.3	60	120	27.4	63.1	43.4

108	0.8	0.2	60	120	25.8	65.8	39.2
109	0.9	0.1	60	120	23.7	48.6	48.7
110	1	0	60	120	20.5	39.2	52.2
112	0	1	15	80	30.9	42.1	73.3
113	0.1	0.9	15	80	30.9	43.0	75.6
114	0.2	0.8	15	80	31.0	47.1	65.8
115	0.3	0.7	15	80	28.9	38.2	75.6
116	0.4	0.6	15	80	29.1	43.5	66.8
117	0.5	0.5	15	80	22.0	22.8	96.4
118	0.6	0.4	15	80	29.5	42.9	68.7
119	0.7	0.3	15	80	27.0	33.2	81.3
120	0.8	0.2	15	80	21.0	23.5	89.3
121	0.9	0.1	15	80	15.4	18.0	85.5
122	1	0	15	80	7.0	9.0	77.7
123	0	1	15	90	31.1	50.8	61.2
124	0.1	0.9	15	90	30.8	51.3	60.0
125	0.2	0.8	15	90	24.7	57.4	43.0
126	0.3	0.7	15	90	30.9	43.7	70.7
127	0.4	0.6	15	90	26.6	64.7	41.1
128	0.5	0.5	15	90	28.3	36.0	78.6
129	0.6	0.4	15	90	30.7	50.8	60.4
130	0.7	0.3	15	90	28.2	44.2	63.8
131	0.8	0.2	15	90	25.8	34.8	74.1
132	0.9	0.1	15	90	19.8	24.5	80.8
133	1	0	15	90	13.7	14.1	97.1
134	0	1	15	100	31.1	51.2	60.7
135	0.1	0.9	15	100	30.1	53.4	56.3
136	0.2	0.8	15	100	29.4	58.3	50.4
137	0.3	0.7	15	100	29.7	52.0	57.1
138	0.4	0.6	15	100	30.7	53.4	57.4
139	0.5	0.5	15	100	30.3	42.5	71.2
140	0.6	0.4	15	100	32.0	48.2	66.3
141	0.7	0.3	15	100	28.7	49.1	58.4
142	0.8	0.2	15	100	27.3	35.4	77.1
143	0.9	0.1	15	100	20.2	24.5	82.4
144	1	0	15	100	17.0	18.2	93.4
145	0	1	15	110	29.8	55.3	53.8
146	0.1	0.9	15	110	19.7	56.4	34.9
147	0.2	0.8	15	110	28.8	58.3	49.3
148	0.3	0.7	15	110	30.0	54.2	55.3
149	0.4	0.6	15	110	28.5	60.4	47.1
150	0.5	0.5	15	110	30.1	44.8	67.1
151	0.6	0.4	15	110	29.3	57.7	50.7
152	0.7	0.3	15	110	28.9	54.9	52.6
153	0.8	0.2	15	110	29.6	44.6	66.3
154	0.9	0.1	15	110	21.4	30.2	70.8
155	1	0	15	110	19.9	27.8	71.5
156	0	1	15	130	27.3	59.5	45.8
157	0.1	0.9	15	130	27.1	60.4	44.8
158	0.2	0.8	15	130	27.7	60.0	46.1
159	0.3	0.7	15	130	27.4	59.4	46.1
160	0.4	0.6	15	130	26.3	64.7	40.6
161	0.5	0.5	15	130	28.3	52.1	54.3
162	0.6	0.4	15	130	27.0	63.1	42.7
163	0.7	0.3	15	130	27.5	61.5	44.7
164	0.8	0.2	15	130	29.3	55.9	52.4
165	0.9	0.1	15	130	26.2	41.2	63.5
166	1	0	15	130	24.9	38.0	65.5

167	0	1	15	140	26.8	61.2	43.7
168	0.1	0.9	15	140	25.3	63.2	40.0
169	0.2	0.8	15	140	24.8	68.7	36.0
170	0.3	0.7	15	140	27.0	60.5	44.6
171	0.4	0.6	15	140	25.9	65.0	39.8
172	0.5	0.5	15	140	30.0	48.4	61.9
173	0.6	0.4	15	140	26.7	61.9	43.1
174	0.7	0.3	15	140	26.9	64.3	41.8
175	0.8	0.2	15	140	28.8	57.3	50.2
176	0.9	0.1	15	140	25.6	56.5	45.3
177	1	0	15	140	24.6	56.1	43.8

The second-order polynomial regression model equations after omitting the highly correlated variables with other *x* variables are:

$$\text{Fructose yield (\%)} = 29.3 - 0.0173\times\text{MgO conc.} - 0.345 \times \text{Time} - 0.009 \times \text{Temp} - 0.112 \times (\text{MgO conc.})^2 - 0.0281\times (\text{Time})^2 - 0.284 \times (\text{Temp})^2 - 0.0025 \times (\text{MgO conc.} \times \text{Time})^2 + 0.216 \times (\text{MgO conc.} \times \text{Temp})^2 \qquad \text{------- (S9)}$$

$$\text{Fructose selectivity (\%)} = 53.6 + 1.58 \times\text{MgO conc.} - 1.64 \times \text{Time} - 4.65 \times \text{Temp} - 0.336 \times (\text{MgO conc.})^2 + 0.196 \times (\text{Time})^2 + 0.376 \times (\text{Temp})^2 - 0.292 \times (\text{MgO conc.} \times \text{Time})^2 - 0.502 \times (\text{MgO conc.} \times \text{Temp})^2 \qquad \text{------- (S10)}$$

$$\text{Glucose conversion (\%)} = 55.6 - 1.22 \times\text{MgO conc.} + 1.14 \times \text{Time} + 3.73 \times \text{Temp} + 0.113 \times (\text{MgO conc.})^2 - 0.167 \times (\text{Time})^2 - 0.437\ \text{DD} + 0.239 \times (\text{MgO conc.} \times \text{Time})^2 + 0.469 \times (\text{MgO conc.} \times \text{Temp})^2 \qquad \text{------- (S11)}$$

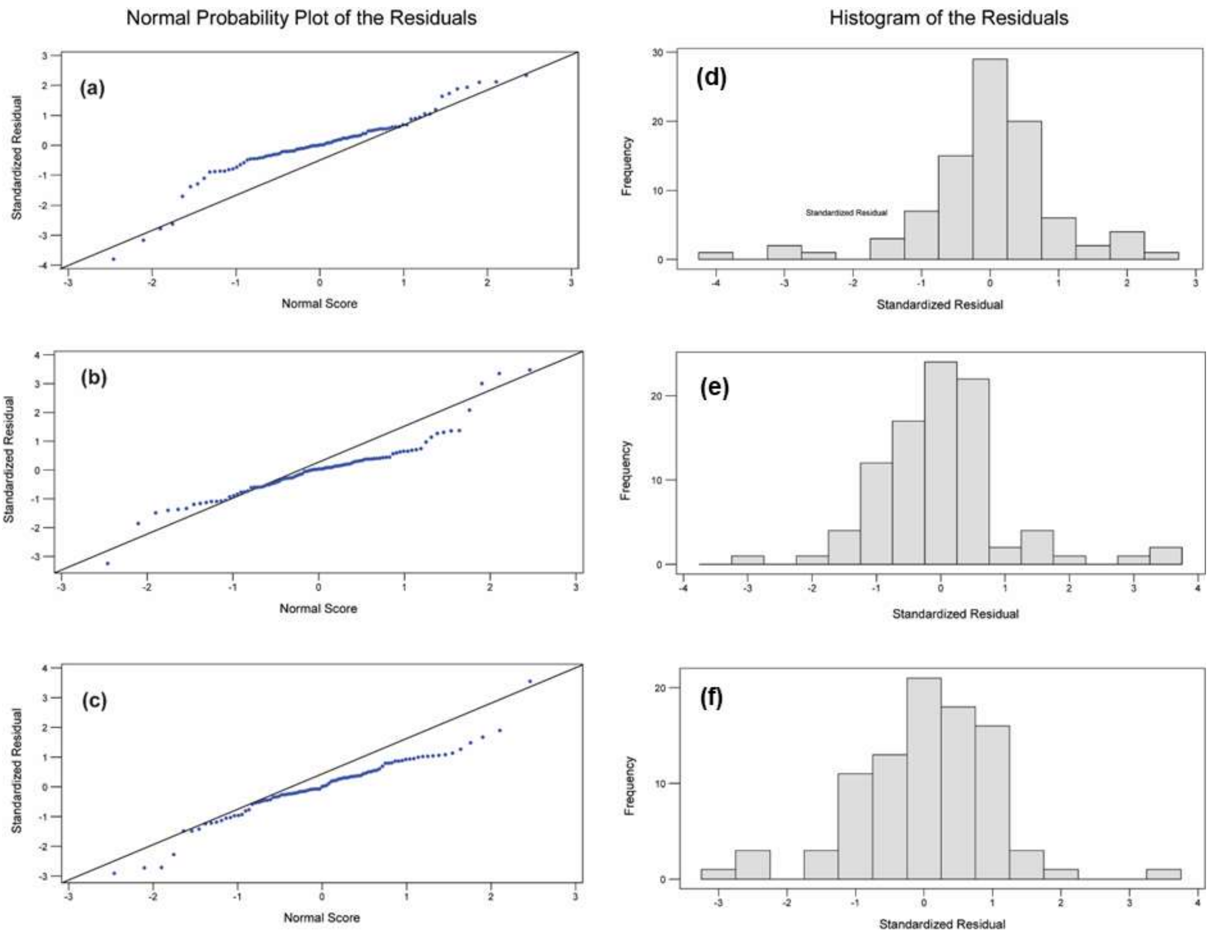

Fig. S13. ANOVA report of normal probability of model-fit residuals and its histogram of fructose yield (a&d), fructose selectivity (b&e) and glucose conversion (c&f).

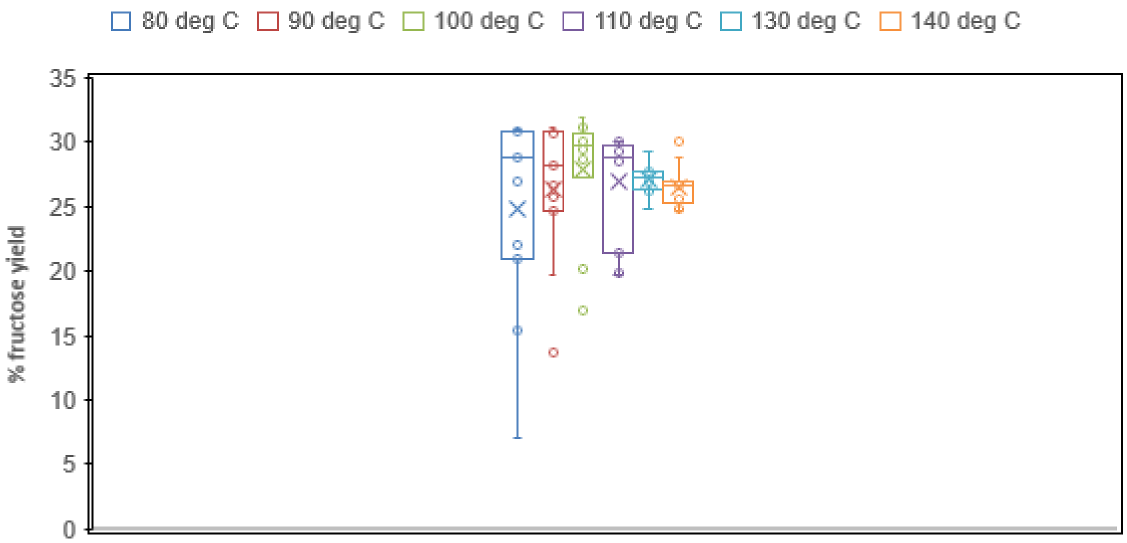

Fig. S14. Box-Wishker plot of fructose yield data obtained using different ratios of MgO/CaO after 15 min.

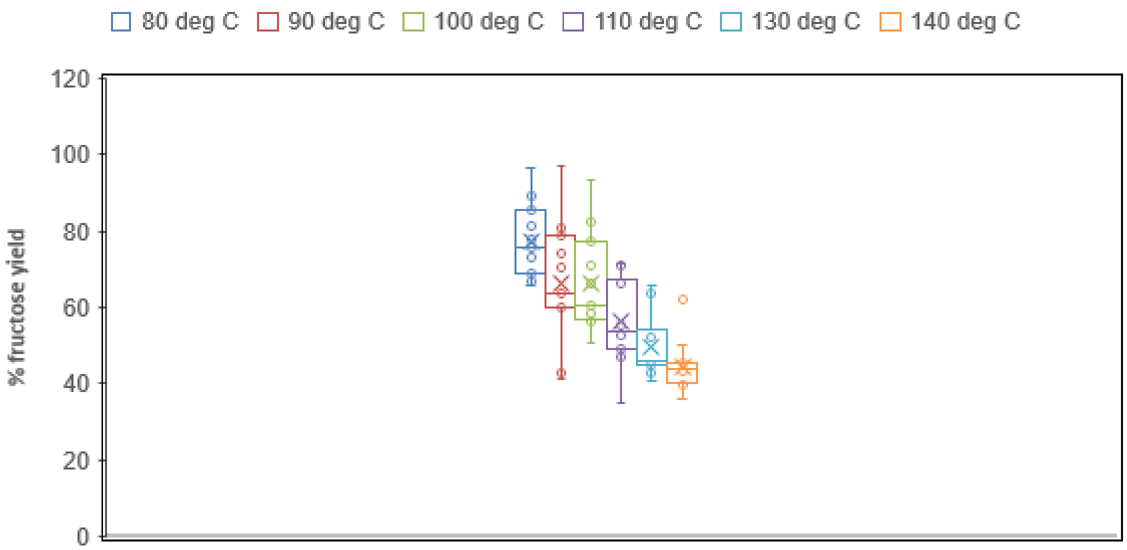

Fig. S15. Box-Wishker plot of fructose selectivity data obtained using different ratios of MgO/CaO after 15 min.

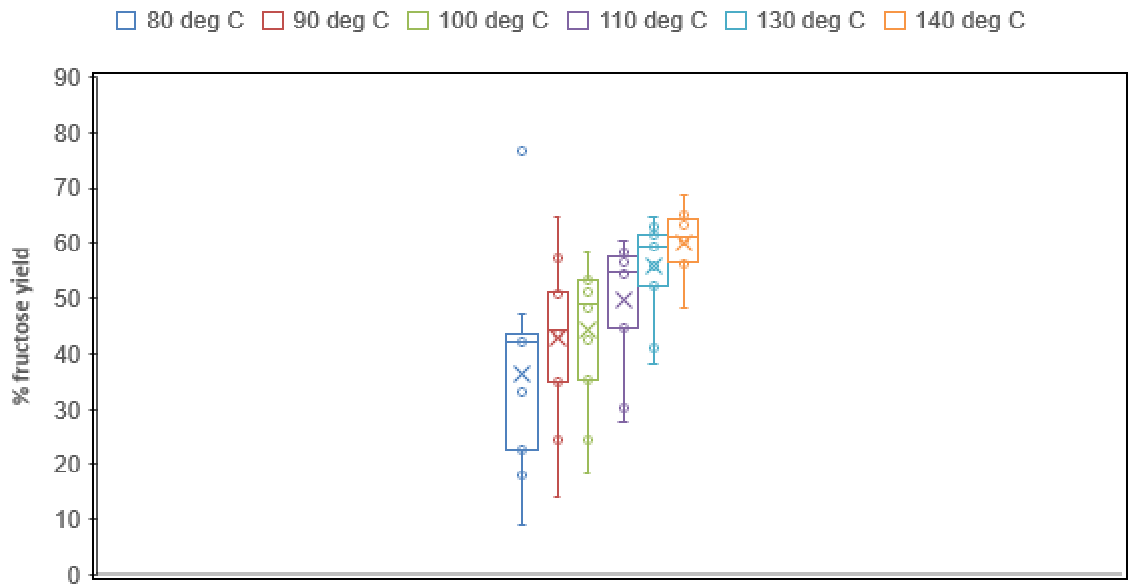

Fig. S16. Box-Wishker plot of glucose conversion data obtained using different ratios of MgO/CaO after 15 min.

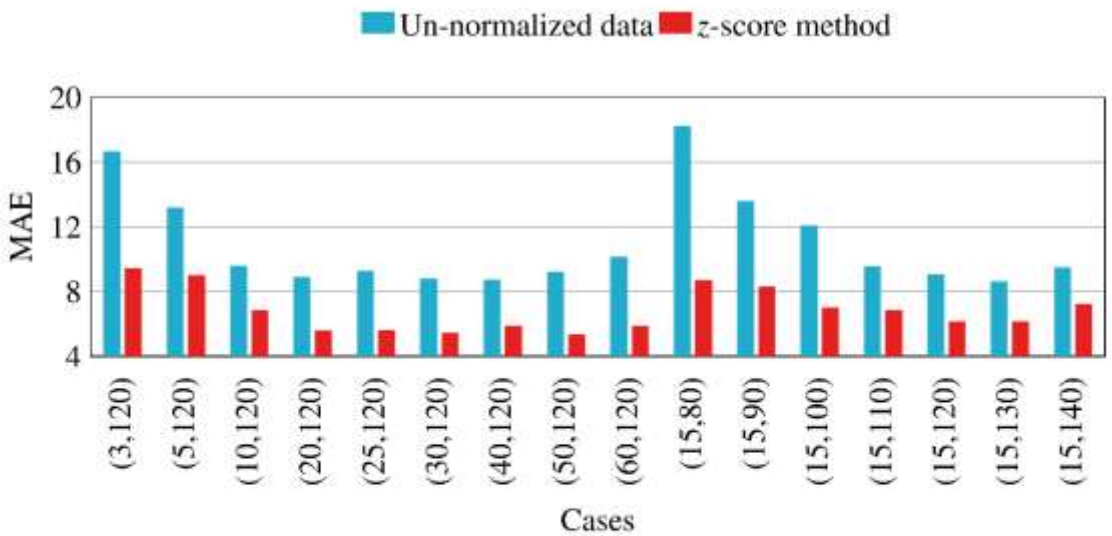

Fig. S17. Impact of data normalization on the prediction of output variables

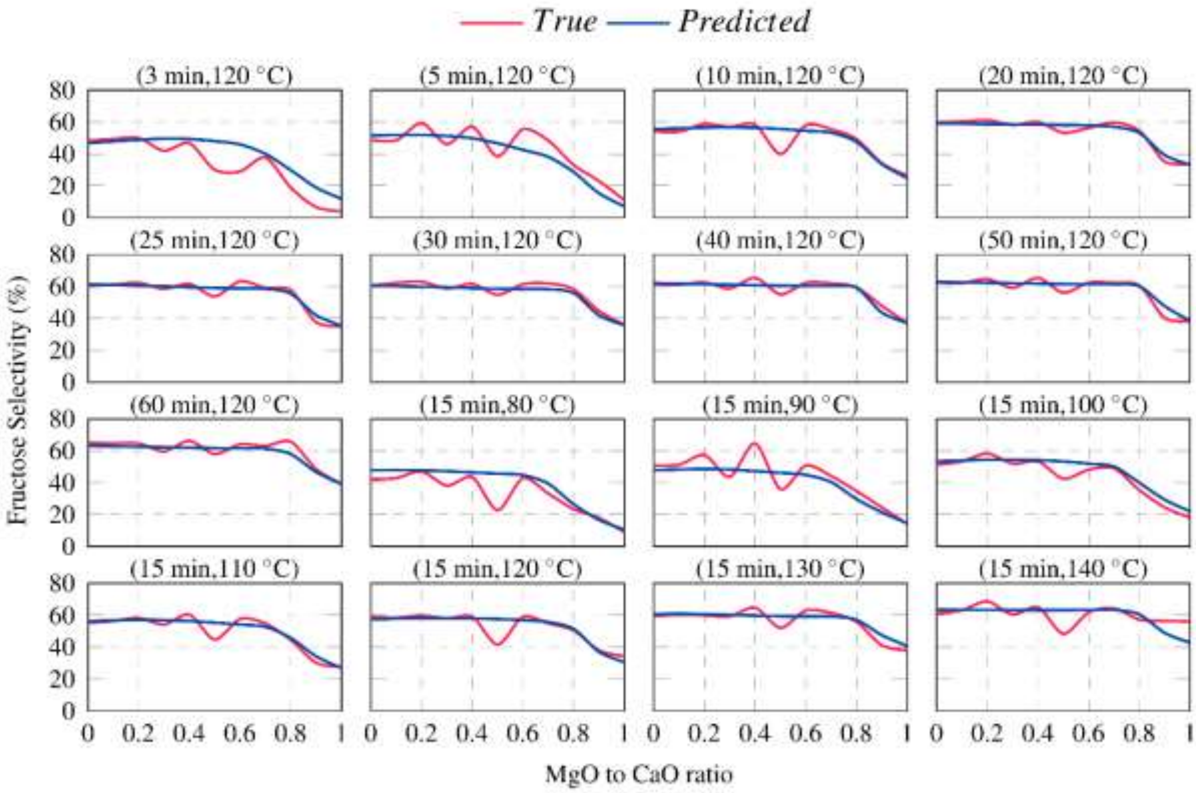

Fig. S18. Comparative modeling result of fructose selectivity over MgO/CaO (at different concentrations of 0 to 100%) using deep neural networks

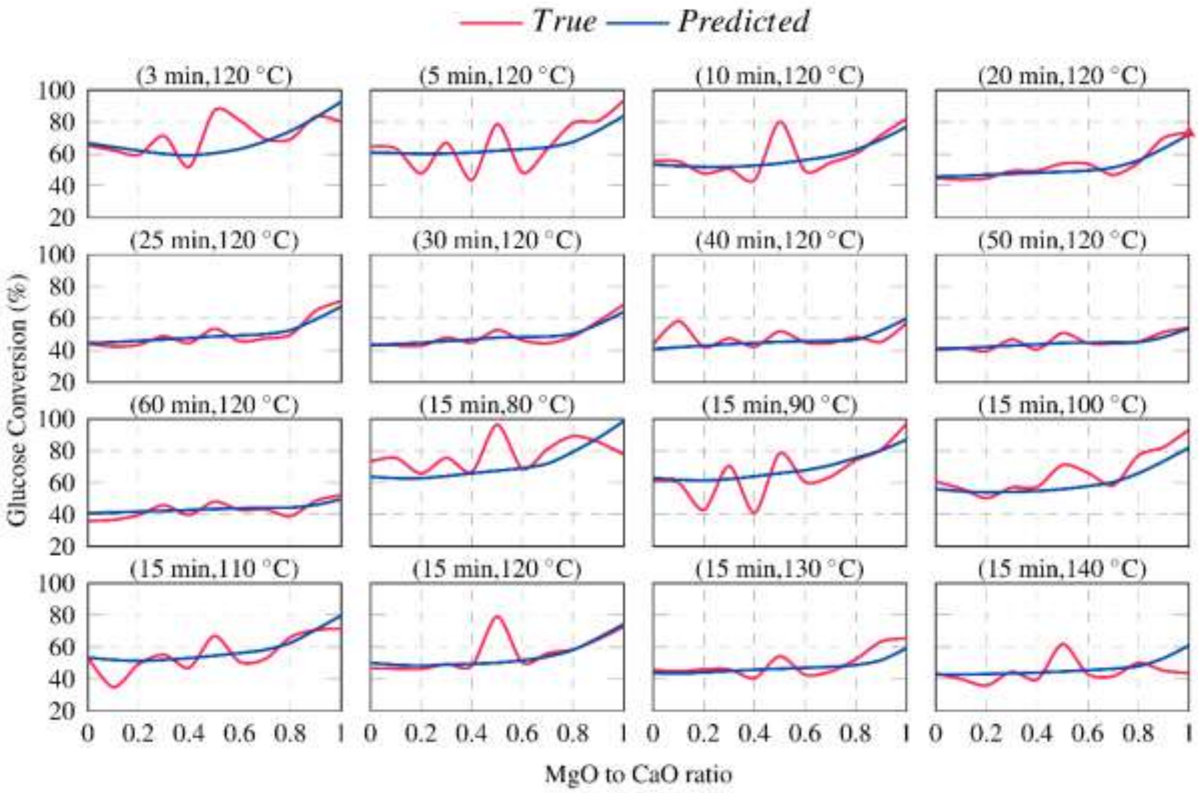

Fig. S19. Comparative modeling result of glucose conversion over MgO/CaO (at different concentrations of 0 to 100%) using deep neural networks

Table S6. Comparison of deep neural network and GLM (Gaussian-Log) for the prediction of fructose yield, fructose selectivity and glucose conversion

Time	Temp.	Deep neural network						Gaussian - Log					
		MAE			R^2			MAE			R^2		
		Yield	Selec.	Conv.	Yield	Selec.	Conv.	Yield	Selec.	Conv.	Yield	Selec.	Conv.
3	120	4.63	7.52	8.12	0.51	0.64	-0.16	6.24	15.96	11.57	-0.05	-0.45	-0.66
5	120	2.70	6.64	9.31	0.68	0.74	0.48	3.56	10.27	12.39	0.33	0.29	0.20
10	120	1.47	3.00	6.10	0.61	0.77	0.48	2.25	7.50	8.72	-0.08	0.41	0.35
20	120	0.97	2.02	2.86	0.64	0.93	0.87	2.50	6.00	4.38	-1.42	0.45	0.66
25	120	0.71	2.16	3.06	0.65	0.92	0.86	2.13	6.32	4.79	-1.56	0.33	0.57
30	120	0.77	2.20	2.40	0.23	0.90	0.87	2.11	5.46	3.90	-2.98	0.26	0.57
40	120	0.69	2.08	4.20	0.88	0.88	-0.24	2.22	5.77	5.35	0.04	0.25	-0.73
50	120	0.68	2.26	1.93	0.82	0.87	0.66	2.39	7.02	3.93	-0.07	0.29	-0.12
60	120	0.87	2.77	3.22	0.76	0.83	0.50	2.43	8.38	6.18	-1.05	-0.36	-0.85
15	80	2.13	5.51	9.95	0.80	0.55	-1.00	4.29	8.15	7.95	0.23	0.27	-0.21
15	90	1.66	5.92	8.44	0.83	0.72	0.51	3.32	9.37	10.01	0.37	0.30	0.30
15	100	1.11	3.53	6.55	0.91	0.87	0.61	3.50	7.11	6.42	0.28	0.51	0.63
15	110	1.75	2.87	5.89	0.40	0.86	0.50	3.22	7.05	6.87	0.02	0.39	0.31
15	120	1.19	2.69	4.06	0.45	0.69	0.33	2.80	5.80	5.66	-1.28	0.47	0.44
15	130	0.63	2.90	4.37	0.38	0.81	0.55	1.86	5.77	4.96	-2.86	0.24	0.30
15	140	0.98	4.89	6.16	0.40	-0.69	-0.67	2.36	7.52	8.42	-2.09	-1.44	-1.19
Win/Loss/Draw		-	-	-	-	-	-	16/0/0	16/0/0	14/2/0	16/0/0	16/0/0	13/3/0

Table S7. Comparison of neural networks and GLM (Gaussian-Identity) for the prediction of fructose yield, fructose selectivity and glucose conversion

Time	Temp.	Neural Networks						Gaussian - Identity					
		MAE			R^2			MAE			R^2		
		Yield	Selec.	Conv.	Yield	Selec.	Conv.	Yield	Selec.	Conv.	Yield	Selec.	Conv.
3	120	4.63	7.52	8.12	0.51	0.64	-0.16	6.21	15.82	12.26	-0.04	-0.35	-0.78
5	120	2.70	6.64	9.31	0.68	0.74	0.48	3.53	9.88	12.8	0.35	0.38	0.12
10	120	1.47	3.00	6.10	0.61	0.77	0.48	2.25	7.27	8.92	-0.09	0.44	0.32
20	120	0.97	2.02	2.86	0.64	0.93	0.87	2.56	5.48	4.91	-1.48	0.50	0.61
25	120	0.71	2.16	3.06	0.65	0.92	0.86	2.18	5.83	5.10	-1.67	0.40	0.50
30	120	0.77	2.20	2.40	0.23	0.90	0.87	2.15	5.02	4.23	-3.19	0.34	0.47
40	120	0.69	2.08	4.20	0.88	0.88	-0.24	2.18	5.72	5.96	0.03	0.32	-1.03
50	120	0.68	2.26	1.93	0.82	0.87	0.66	2.46	6.98	3.83	-0.13	0.26	-0.13
60	120	0.87	2.77	3.22	0.76	0.83	0.50	2.52	8.13	6.92	-1.28	-0.33	-1.35
15	80	2.13	5.51	9.95	0.80	0.55	-1.00	4.29	7.04	7.76	0.26	0.51	-0.06
15	90	1.66	5.92	8.44	0.83	0.72	0.51	3.33	8.46	10.48	0.39	0.38	0.21
15	100	1.11	3.53	6.55	0.91	0.87	0.61	3.48	6.18	7.20	0.30	0.63	0.55
15	110	1.75	2.87	5.89	0.40	0.86	0.50	3.19	6.49	7.14	0.02	0.46	0.23
15	120	1.19	2.69	4.06	0.45	0.69	0.33	2.87	5.49	5.95	-1.33	0.49	0.43
15	130	0.63	2.90	4.37	0.38	0.81	0.55	1.95	5.56	4.98	-3.14	0.24	0.31
15	140	0.98	4.89	6.16	0.40	-0.69	-0.67	2.43	7.75	7.71	-2.28	-1.72	-0.93
Win/Loss/Draw		-	-	-	-	-	-	16/0/0	-	-	-	-	-

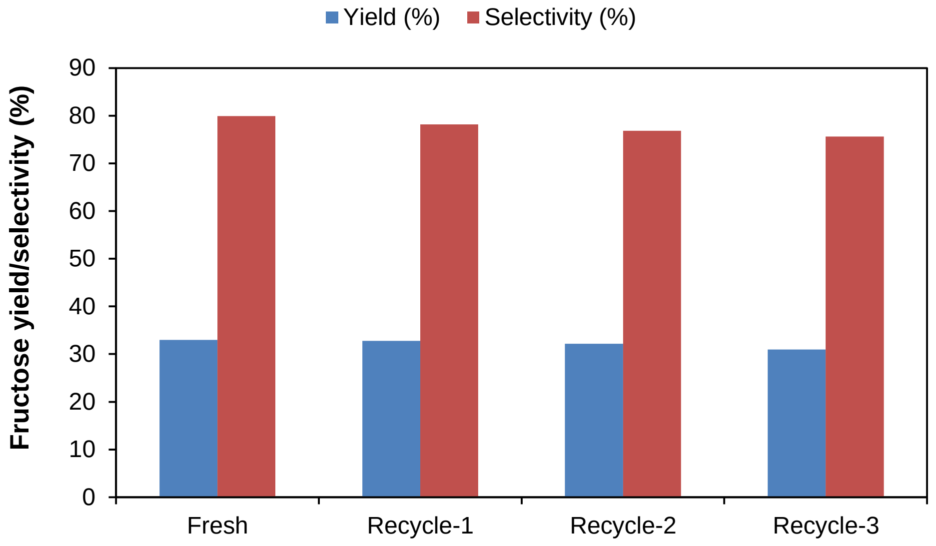

Fig. S20. Performance result of MC-A during recycling under the optimum reaction conditions when using glucose.

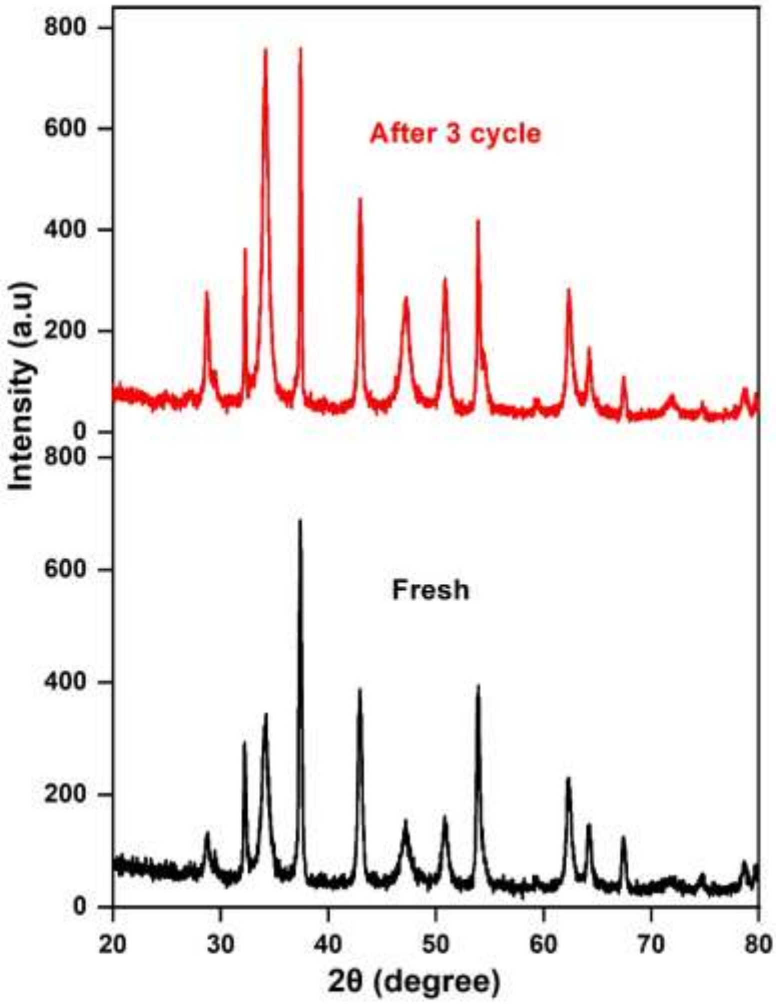

Fig. S21. Comparative XRD result of MC-A before and after 3 recycles.

Table S8. FOB cost of purchased equipment(s) for glucose to product(s)-CAPEX[a]

Equipment (Major)	**Operating capacity**	**No. of Units**	**Unit price (USD)**	**Cost (USD)**
Batch reactor	30 kilo Lit/h	1	$1,50,990	$1,50,990
Storage tank	30 m^3	1	$17,955	$17,955
Distillation column	1 ton/h	1	$10,00,000	$10,00,000
Multiple hearth furnace	1 ton/h	1	$39,03,318	$39,03,318
Batch reactor	10 kLit/h	1	$77,989	$77,989
Centrifuge	10 kLit/h	2	$63,489	$1,26,978
Dryer	1 ton/h	1	$1,25,919	$1,25,919
Packed bed column	1 ton/h	1	$10,00,000	$10,00,000
Small, low pressure seed tank	10 m^3	4	$9,236	$36,944
			Total	$64,40,093
Component		**Suggested factor**		**Cost (USD)**
Purchased equipment (FOB, delivered): PE		Same total	-	$64,40,093
Installation		0.25% of PE	-	$16,10,023
Instrumentation		0.25% of PE	-	$16,10,023
Piping		0.1% of PE	-	$6,44,009
Electrical		0.1% of PE	-	$6,44,009
Building		0.15% of PE	-	$9,66,014
Yard improvements		0.12% of PE	--	$7,72,811
Service facilities		0.25% of PE	-	$16,10,023
Total direct plant cost, D				$1,42,97,006
Engineering and supervision		0.25% of PE	-	$16,10,023
Construction expenses		0.25% of PE	-	$16,10,023
Legal expenses		0.04% of PE	-	$2,57,604
Contractor's fee		0.05% of PE	-	$3,22,005
Contingency		0.01% of PE	-	$64,401
Total indirect plant cost, I				$38,64,056
Fixed-capital investment (FCI), D+I				$1,81,61,062
Working capital (13% TCI)				$27,24,159
Total capital investment (TCI)				**$2,08,85,222**

[a]The rates of the equipment(s) were obtained using the chemical engineering cost index data. The scaling factor used for estimating the cost of the equipment(s) was 0.6 [1-3].

Table S9. Operating expenses (OPEX) of glucose interconversion to product(s)

Direct production costs	Unit rate	Requirement	Cost (USD)
Raw materials[b,c]			
Glucose	390/ton	1	$390
Silica gel	1000/ton	1	$1,000
Sodium hydroxide	230/ton	0.08	$18
Magnesium sulfate	400/ton	0.12	$48
Calcium hydroxide	60/ton	0.07	$4
Ethanol	899/ton	1	$90
Acetone	725/ton	1	$73
Operating labor (10-employee hr/day): OL	$10/hr	-	$1,09,500
Operating supervision: OS	0.01% of OL	-	$1,095
Utilities			
Steam for drying purposes	4.4/1000 kg	-	$44
Electricity	0.045 kWh	-	$3,240
Fuel	0.35/GJ	-	$50
Refrigeration	20/GJ	-	$1,000
Waste treatment disposal	1.06/ton	-	$382
Water	1/ton	-	$10,000
	Suggested factor		
Maintenance and repairs: MR	0.01% of FCI	-	$1,81,611
Operating supplies	0.01% of MR	-	$1,816
Laboratory charges	0.01% of OL	-	$1,095
Royalties	0.01% of FCI	-	$1,81,611
		Sub-total	$4,93,066
Fixed charges			
Taxes (property)	0.01% of FCI	-	$1,81,611
Financing (interest)	0.001% of FCI	-	$18,161
Insurance	0.01% of FCI	-	$1,81,611
Rent	0.001% of FCI	-	$18,161
Depreciation	0.01% of FCI	-	$2,08,852
		Sub-total	$6,08,396
Plant overhead costs	0.5% of OL&MR		$2,922
		Sub-total	$11,04,383
General expenses			
Administrative costs	0.25% of TPC	-	$58,441
Distribution and marketing	0.02% of TPC	-	$1,169
Research and development	0.05% of TPC	-	$55,219
		Sub-total	$1,14,829
		Total variable production cost	$12,19,212

[b]The rates were obtained from the online-market (www.alibaba.com/).
[c] Based on the actual supply (recovery and reuse).

Table S10. Other cost parameters and assumptions of glucose to product(s)[c] [4, 5]

Item description	Value
Plant operation	Continuous
Plant life	30 years
Total revenue ($/yr) (including fructose, allulose and mannose)	3,468,966
Interest rate	8%
Tax rate	30%
Capital recovery factor	0.09
Return on investment	12%
Net annual profit ($)	1,098,485
Depreciation period	10 years

[c]Break-even point: Total revenue = total production cost + ROI + income tax
[d]The depreciation amount was calculated by using the straight-line method for 10 years.

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