Supporting Information

Complete conversion of lignocellulosic biomass to mixed organic acids and ethylene glycol via cascade steps

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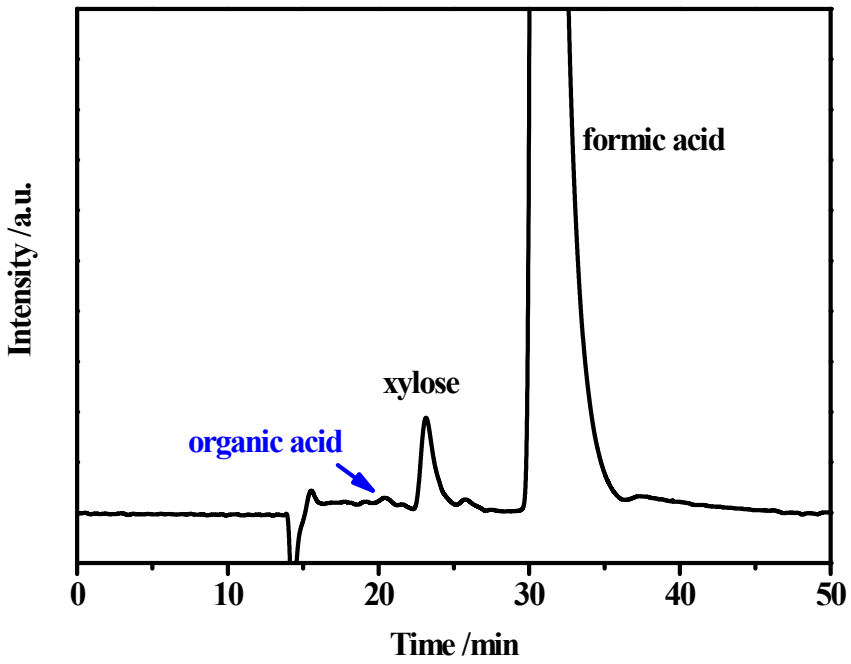


Fig. S1 The HPLC profile of liquid products diluted with water.

Table S1 Effect of H_2O_2 amounts on lignin conversion[a]

Amount of H_2O_2 /%	**Yield /% (Based on NPOC)[b]**
0	40.6
2	57.3
4	86.7
8	95.0

[a] reaction conditions: 0.2 g lignin, 10 mL formic acid and certain amounts of 30% H_2O_2, 353 K; [b] after reaction, the solid was filtered and the formic acid was removed by the evaporation method for total organic carbon measurement.

Table S2 Conversion of lignin in the solvent of acetic acid.[a]

H_2O_2 amount/ mL	conversion /%	formic acid yield /%

0.5	100	0.42
1	100	0.56
2	100	0.61

[a] 0.2 g lignin, 10 mL formic acid and certain amounts of 30% H_2O_2 at 353 K.

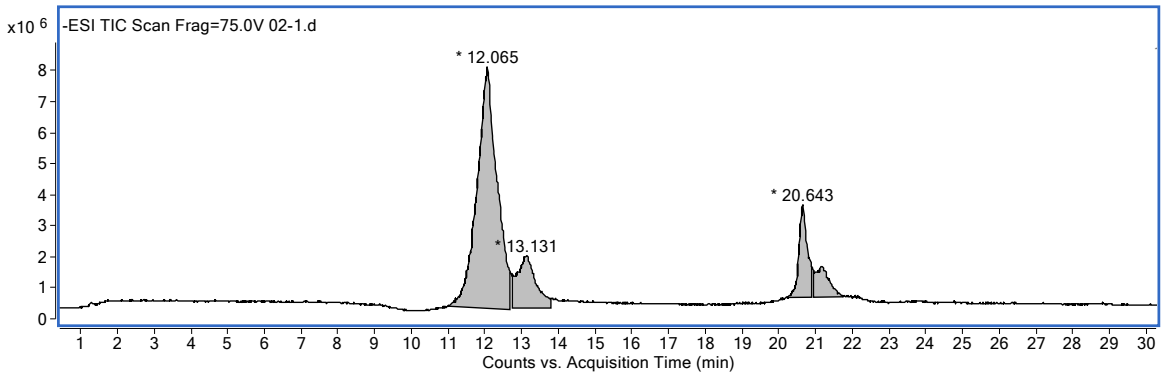


Fig. S2 The HPLC-MS profile of lignin conversion products.

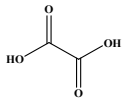
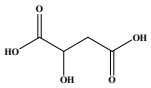
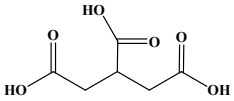
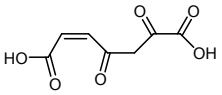
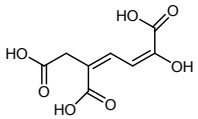
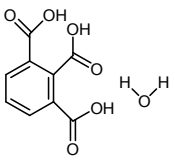
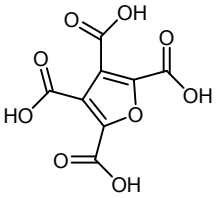
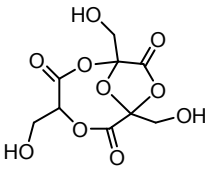
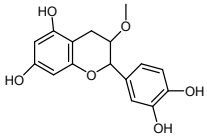
Table S3 Lignin conversion products in Figure S2

Formula	Best	Mass	Tgt Mass	Ion Species	Score
Peak at 12.065 min					
C3H4O2	TRUE	72.0212	72.0211	C3H3O2	97.96
C3H4O4	TRUE	104.0108	104.011	C3H3O4	87.54
C4H4O4	TRUE	116.0109	116.011	C4H3O4	99.84
C5H6O4	TRUE	130.0264	130.0266	C5H5O4	95.56
C6H6O4	TRUE	142.0263	142.0266	C6H5O4	99.4
C5H6O5	TRUE	146.0213	146.0215	C5H5O5	99.21
C7H6O6	TRUE	186.0163	186.0164	C7H5O6	95.85
Peak at 13.131 min					
C3H6O3	TRUE	90.0317	90.0317	C3H5O3	87.87
C4H6O4	TRUE	118.0265	118.0266	C4H5O4	99.73
C4H8O3	TRUE	104.0472	104.0473	C4H7O3	87.64

C4H6O5	TRUE	134.0215	134.0215	C4H5O5	99.99
C5H8O5	TRUE	148.0373	148.0372	C5H7O5	95.38
C8H10O6	TRUE	202.0482	202.0477	C8H9O6	98.96
C9H12O6	TRUE	216.0639	216.0634	C9H11O6	84.91
C6H8O4	TRUE	144.0421	144.0423	C6H7O4	97.57
C7H8O4	TRUE	156.0423	156.0423	C7H7O4	89.75
C7H10O4	TRUE	158.058	158.0579	C7H9O4	96.86
C6H8O6	TRUE	176.0322	176.0321	C6H7O6	93.09
Peak at 20.643 min					
C5H10O4	TRUE	134.0578	134.0579	C5H9O4	97.73
C5H8O4	TRUE	132.0421	132.0423	C5H7O4	87.6
C5H6O4	TRUE	130.0265	130.0266	C5H5O4	99.75
C6H8O4	TRUE	144.0423	144.0423	C6H7O4	81.55
C5H10O5	TRUE	150.0528	150.0528	C5H9O5	76.47
C6H10O6	TRUE	178.0479	178.0477	C6H9O6	89.78
C6H12O6	TRUE	180.0636	180.0634	C6H11O6	85.43
C4H8O4	TRUE	120.0422	120.0423	C4H7O4	87.68
C4H6O4	TRUE	118.0265	118.0266	C4H5O4	87.59
C5H6O3	TRUE	114.0315	114.0317	C5H5O3	99.69
Peak at 21.358 min					
C9H12O5	TRUE	200.0689	200.0685	C9H11O5	82.27
C12H12O7	TRUE	268.0595	268.0583	C12H11O7	85.36
C13H14O9	TRUE	314.0635	314.0638	C13H13O9	89.45
C13H14O8	TRUE	298.0703	298.0689	C13H13O8	89.97
C8H12O3	TRUE	156.0786	156.0786	C8H11O3	99.78
C6H6O4	TRUE	142.0265	142.0266	C6H5O4	87.22
C5H4O4	TRUE	128.0109	128.011	C5H3O4	87.01
C5H10O3	TRUE	118.0629	118.063	C5H9O3	87.68
C4H8O3	TRUE	104.0472	104.0473	C4H7O3	87.35

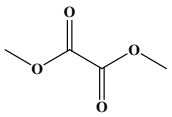
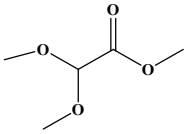
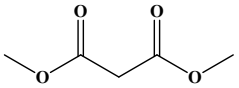
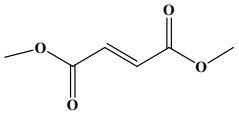
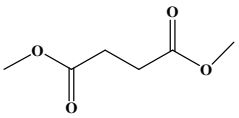
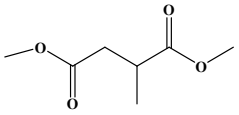
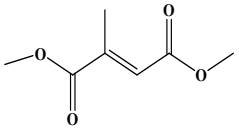
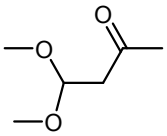
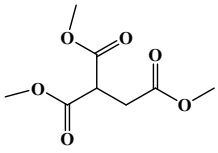
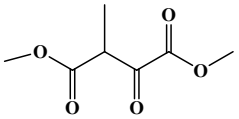
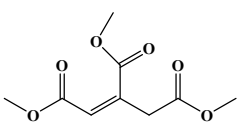
C5H4O2	TRUE	96.021	96.0211	C5H3O2	93.43

Table S4 The chemical structure of typical products in Figure 3 (A)[a]

Code	m/z (1-)	Formula(-H)	structure	CAS#	Name
1-1	88.988	C2H1O2		144-62-7	Oxalic acid
1-2	133.014	C4H5O5		97-67-6	Malic Acid
1-3	175.124	C6H7O6		99-14-9	Tricarballylic acid
1-4	185.009	C7H5O6		5280494 [b]	3-maleylpyruvic acid
1-5	215.020	C8H7O7		21864724 [c]	(2Z,4E)-5-Hydroxy-2,4-pentadiene-1,2,5-tricarboxylic acid
1-6	227.020	C9H7O7		36362-97-7	1,2,3-Benzenetricarboxylic acid hydrate
1-7	242.075	C8H3O9		20416-04-0	Furantetracarboxylic acid
1-8	277.020	C9H9O10		129677010 [b]	Epoxytriglyceride
1-9	303.036	C16H16O6		47610 [b]	3-O-Methylcatechin

[a] the structure of all compounds are determined by the m/z with the deviation of <0.01; [b] the number indicates the PubChem CID; [c] the number indicates the ChemSpider ID.

Table S5 The chemical structure of typical products in Figure 3 (B)

Code	Time	Formula(-H)	structure	CAS#	Name
2-1	4.7	C6H10O4		95-92-1	Diethyl oxalate
2-2	5.4	C5H10O4		89-91-8	Methyl dimethoxyacetate
2-3	6.9	C5H8O4		108-59-8	Dimethyl malonate
2-4	8.8	C6H8O4		624-49-7	Dimethyl fumarate
2-5	9.0	C6H10O4		106-65-0	dimethyl succinate
2-6	9.1	C7H12O4		1604-11-1	Dimethyl methylsuccinate
2-7	9.6	C7H10O4		617-54-9	Dimethyl citraconate
2-8	10.2	C6H12O3		5436-21-5	4,4-Dimethoxy-2-butanone
2-9	13.6	C8H12O6		40967-67-7	Trimethyl ethane-1,1,2-tricarboxylate
2-10	14.7	C7H10O5		264-564-1	Dimethyl 2-methyl-3-oxosuccinate
2-11	15.8	C9H12O6		20820-77-3	Trimethyl aconitate

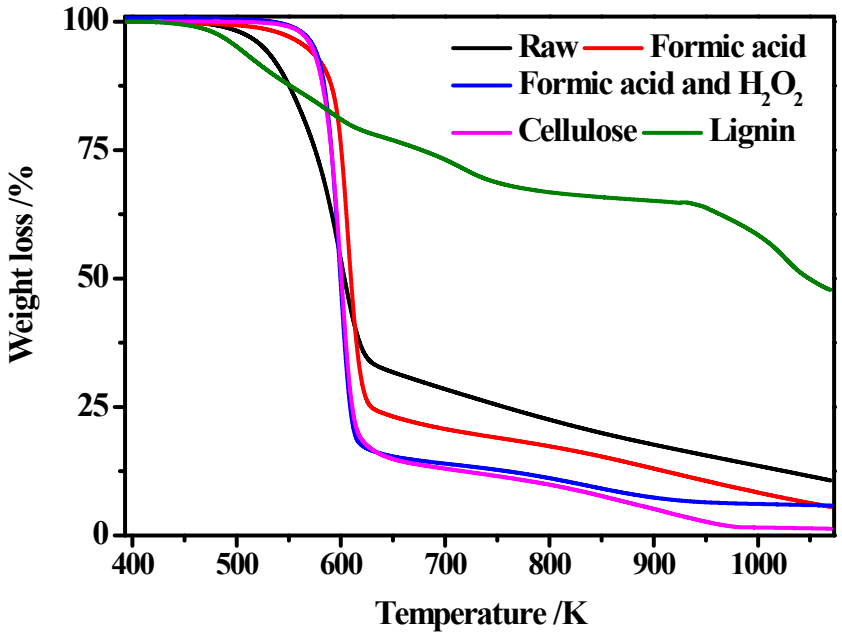


Fig. S3 TG curves of the raw and pretreated Miscanthus.

Table S6 Product distributions after the transformation of different biomass.

Feedstock[a]	Initial weight /g	Hemicellulose and lignin derived products /g		Cellulose derived products /g[b]			Weight balance /%
		maleic acid	others	EG	1,2-PG	others	
Birch wood	10	0.84	3.3	3.8	0.21	1.7	98.5
Miscanthus	10	0.90	4.1	3.2	0.23	1.4	98.3
Corn stalk	10	0.76	4.7	2.6	0.22	1.5	97.8

[a] Corn stalk was washed with water to remove the water-soluble compounds; [b] others was calculated by the equation: Weight of cellulosic biomass = Sum of weights of EG, 1,2-PG and others.