

Supplementary Materials

Figure S1. Solution-state ^1H -NMR spectral analysis of BC degradation products generated in an anaerobic digestion ecosystem. Sampling time is represented by colored lines as indicated in the figure.

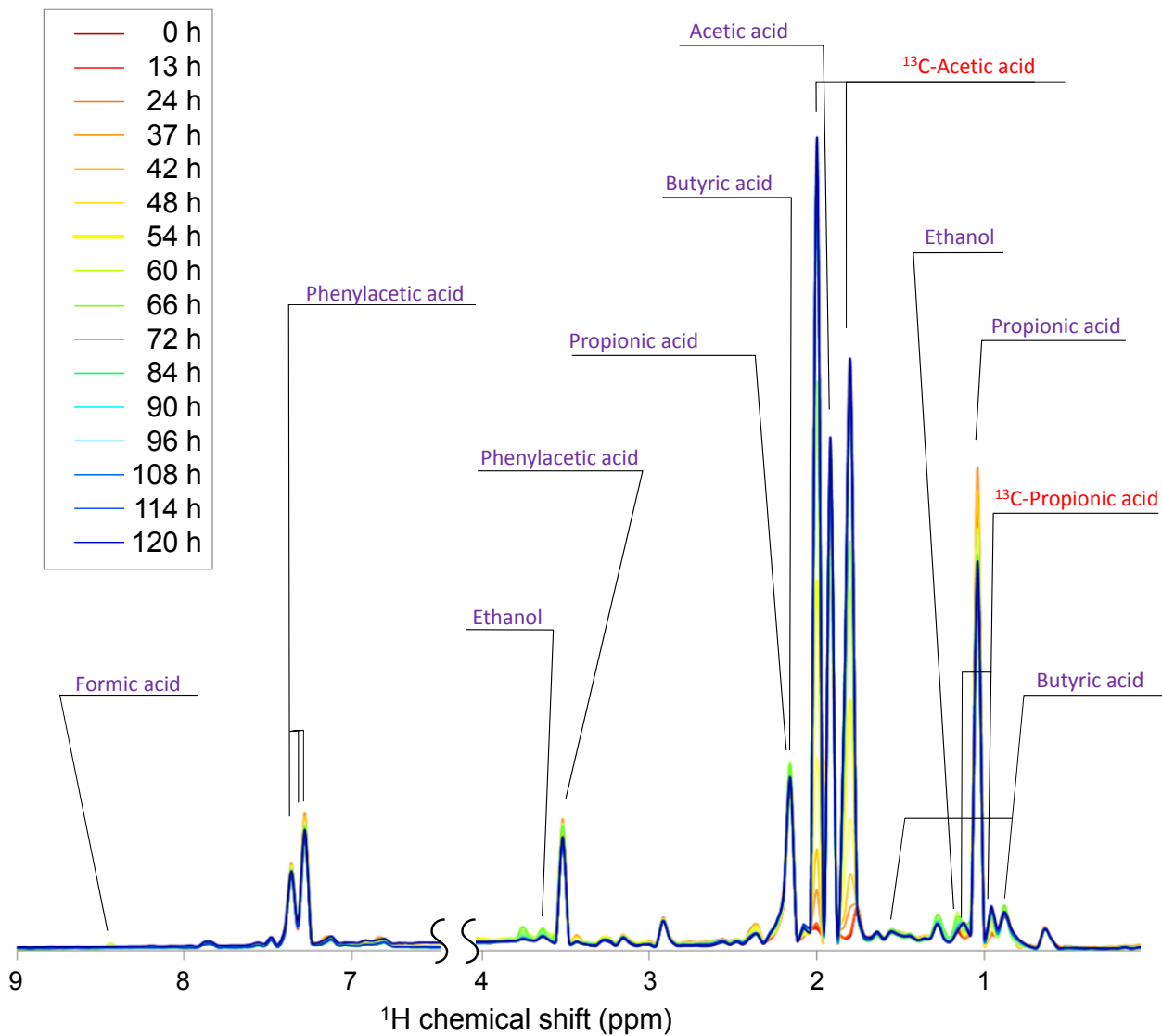


Figure S2. Solution-state ^{13}C -NMR spectral analysis of BC degradation products generated in an anaerobic digestion ecosystem. Sampling time is represented by colored lines as indicated in the figure.

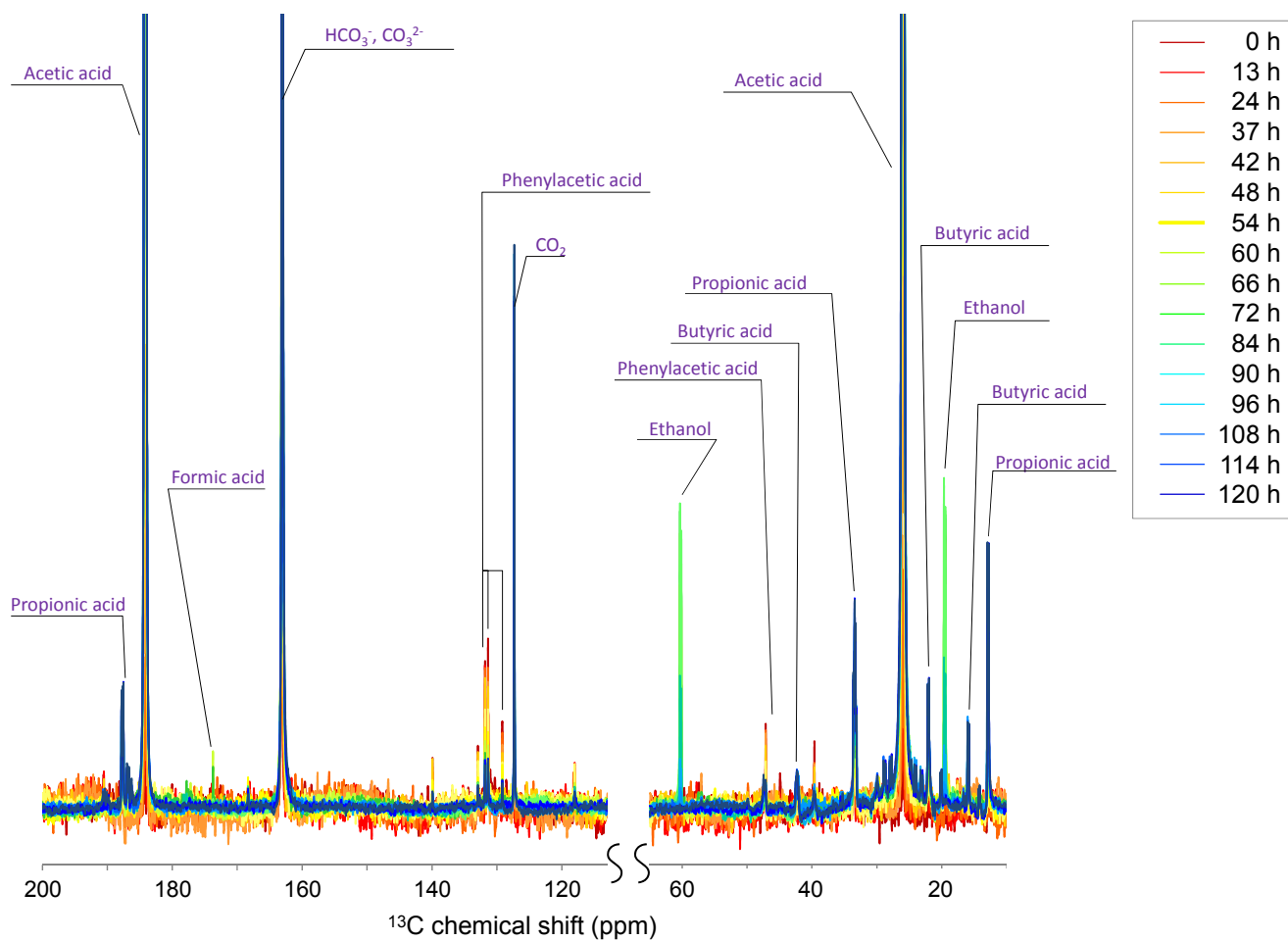


Figure S3. PCA score plot (A) and loading plot (B) of solution-state ^{13}C -NMR spectra. Sampling time is represented by colored lines as indicated in the figure.

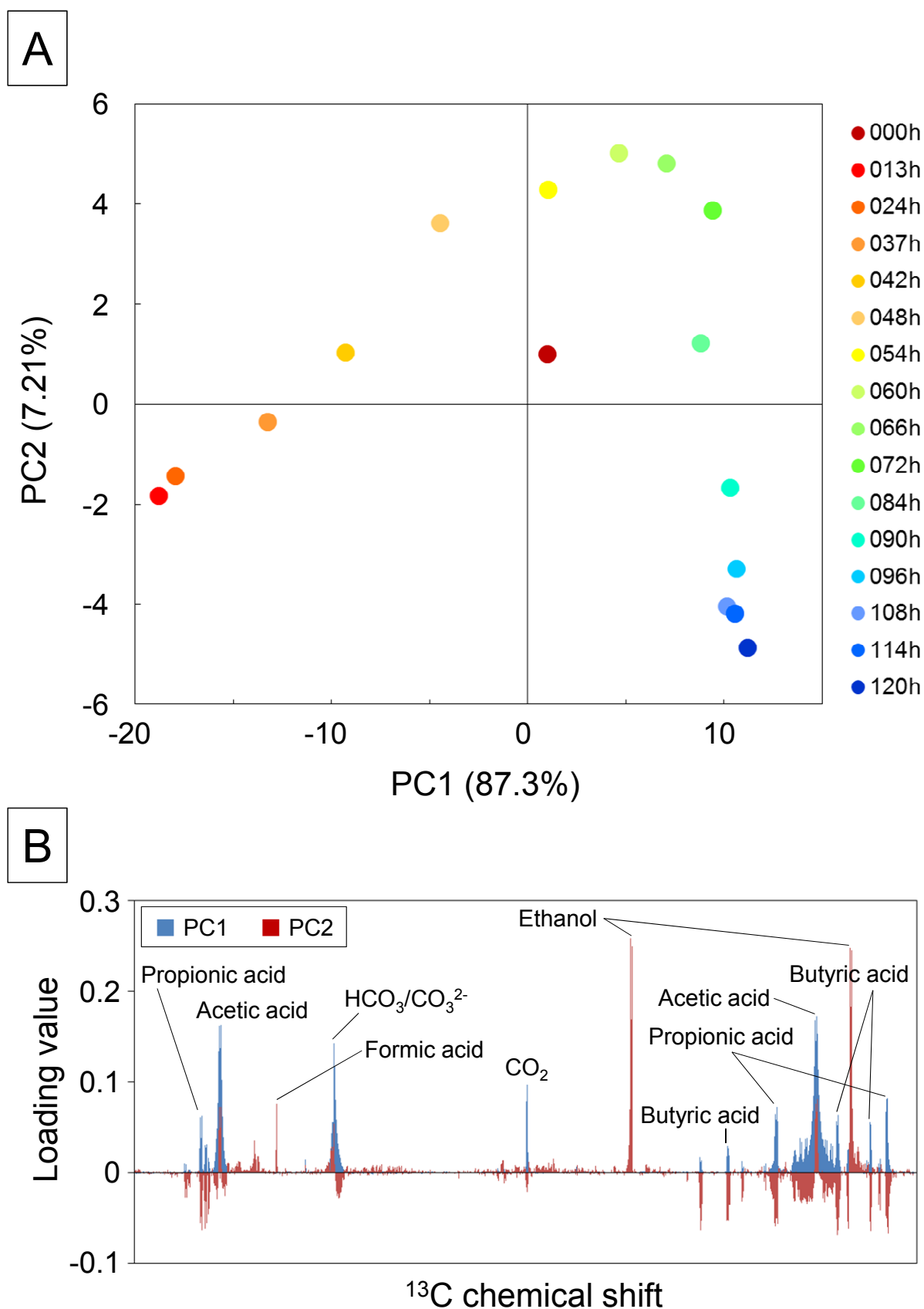


Figure S4. Time course variations of $^{13}\text{C}\text{-HCO}_3^-/\text{CO}_3^{2-}$ and CO_2 intensities observed in solution-state ^{13}C -NMR spectra of BC degradation profiles.

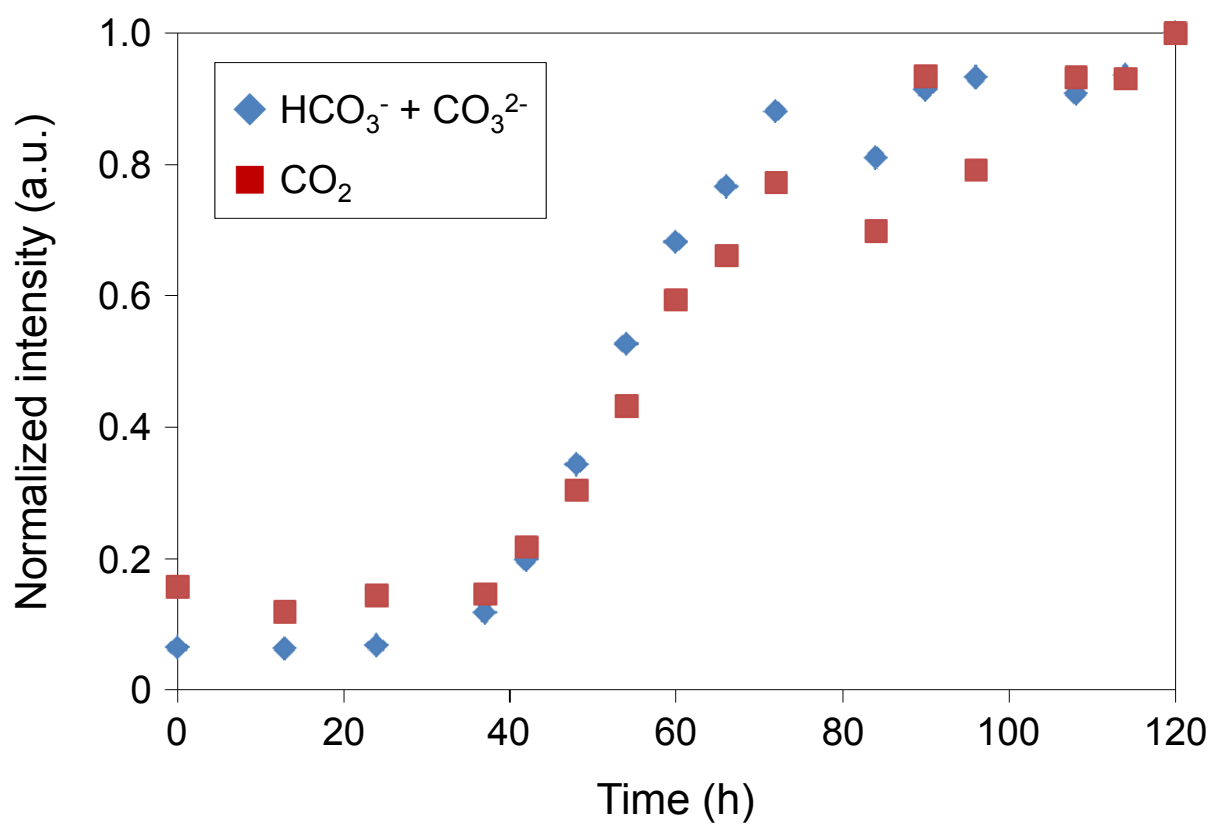


Table S1 Annotated peaks of molecules detected in solid-, solution-, and gas-state NMR spectroscopy.

Substances	¹ H chemical shift ppm (multiplicity)	¹³ C chemical shift ppm (half width(Hz) for CP-MAS)	
Cellulose (solid)			
C1		105.18	
C2, 3, 5		74.68, 71.93	
C4		89.11	
C4'		84.28	
C6		65.38	
C6'		62.55	
Crystalline Iα			
C1		105.01 (179.8)	
C4		89.72 (180.0)	
		88.94 (166.9)	
C6		65.26 (204.0)	
Crystalline Iβ			
C1		105.57 (297.2)	
		104.20 (235.0)	
C4		88.39 (242.1)	
		88.94 (166.9)	
C6		66.03 (144.6)	
		64.62 (245.1)	
para-Crystalline C4			
Accessible fibril surface1	C4	88.96 (573.7)	
Accessible fibril surface2	C4	84.53 (131.2)	
Inaccessible fibril surface	C4	83.21 (297.2)	
	C4	83.83 (940.4)	
Proteins (solid)			
sc		9.84-45.53	
bb		46.84-59.10	
C=O		166.89-183.01	
Lipids (solid)			
(CH ₂) _n		30.39	
Small molecules (liquid)			
Butyric acid	0.874	(t)	15.95
	1.541	(m)	22.08
	2.137	(t)	42.26
	-		186.48
Propionic acid	1.045	(t)	12.91
	2.172	(q)	33.41
	-		187.69
Ethanol	1.172	(t)	19.57
	3.649	(q)	60.23
Acetic acid	1.909	(s)	26.0
	-		184.18
Phenylacetic acid	3.528	(s)	47.12
	7.294	(t)	129.17
	-		131.85
	7.373	(t)	131.37
	-		139.93
	-		183.80
Formic acid	8.443	(s)	173.74
HCO ₃ ⁻ , CO ₃ ²⁻	-		163.13-163.07
CO ₂	-		127.34
Small molecules (gas)			
CO ₂	-		130.47
CH ₄	3.203		-5.53