Electronic Supplementary Information

Molecular Transformation and Metabolic Insights of Microbial Electrolysis Treatment and Valorization of Post-hydrothermal Liquefaction Wastewater

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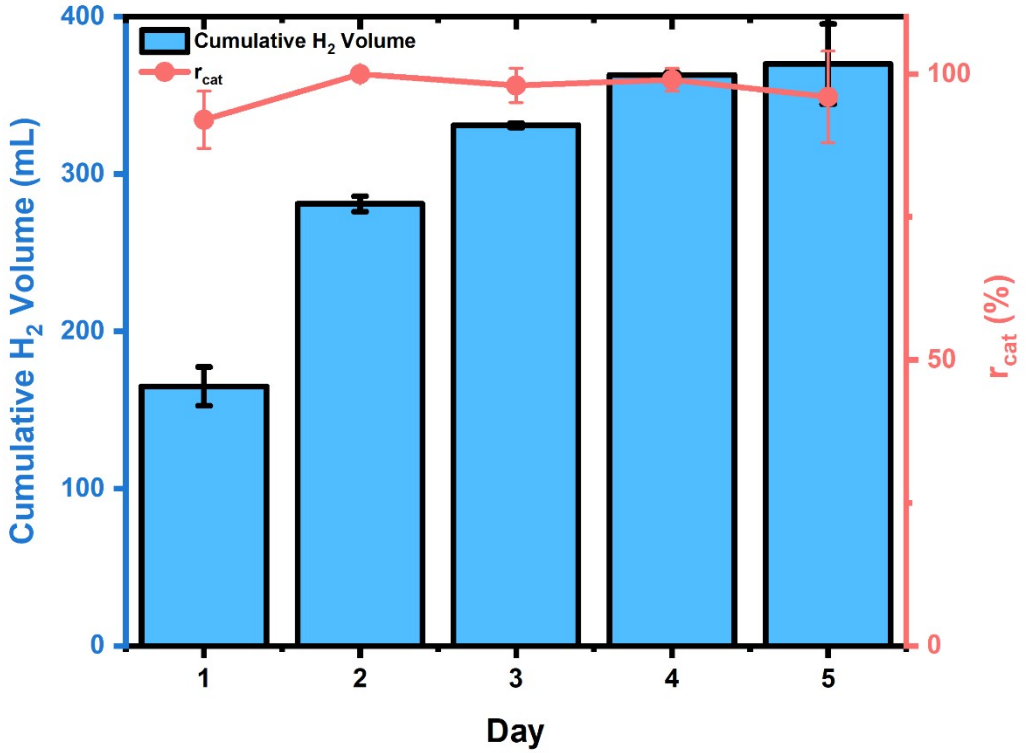


Figure S1. The cumulative H_2 production and cathodic H_2 recovery under the identified optimal condition.

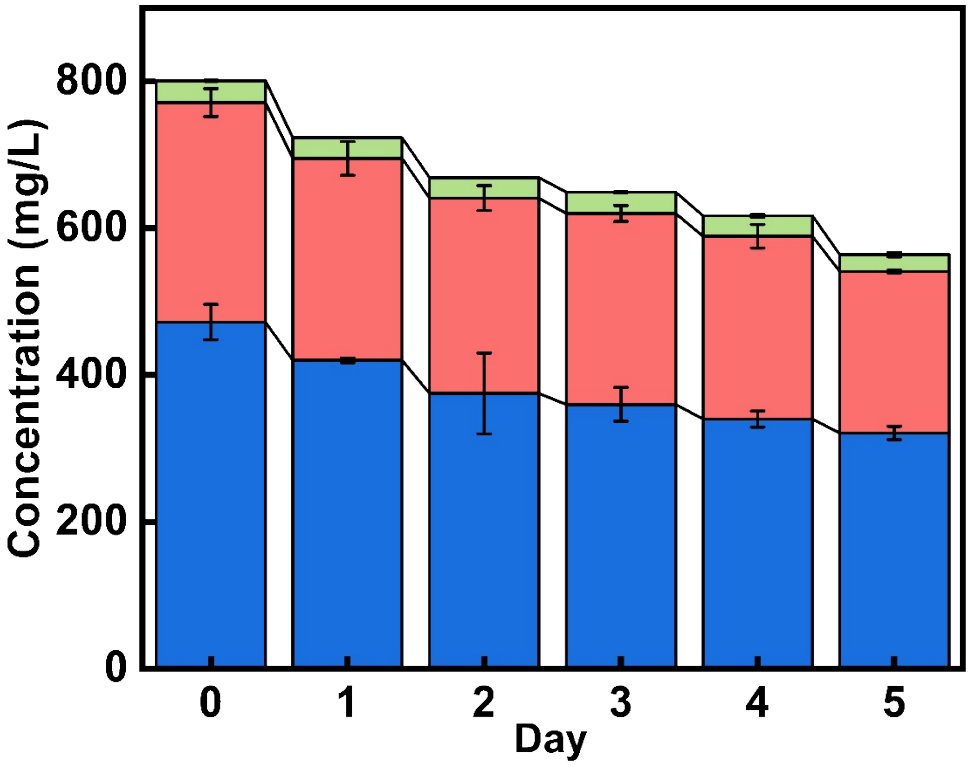


Figure S2. The combined concentration profile of open-circuit control reactors. Blue: alcohols; Red: VFAs; Green: other HPLC-identified chemicals

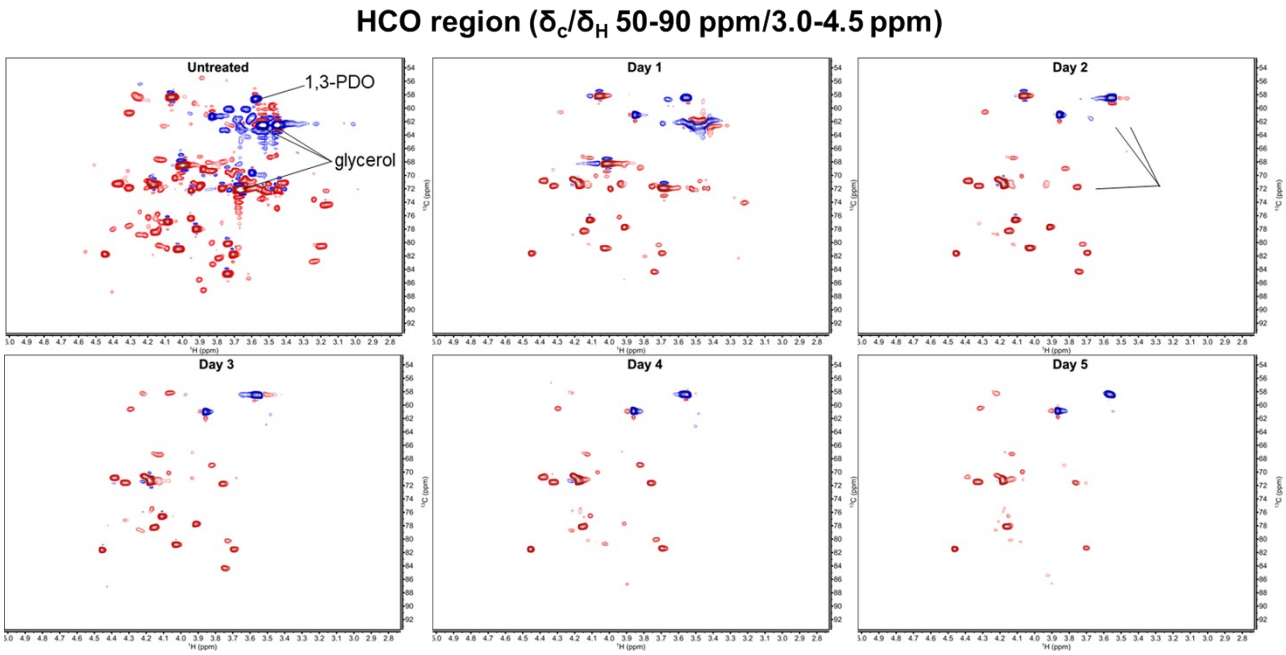


Figure S3. The ^{1}H-^{13}C HSQC NMR zoom-in view of the H_nCO region.

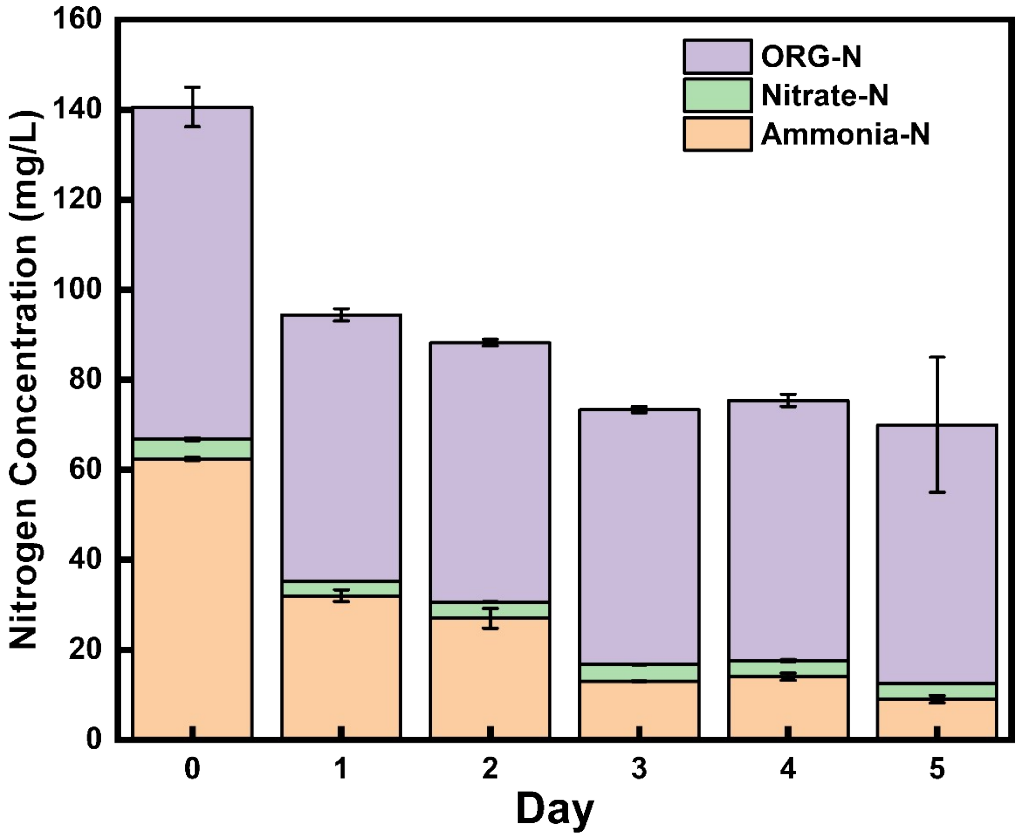


Figure S4. Nitrogen profile during MEC treatment.

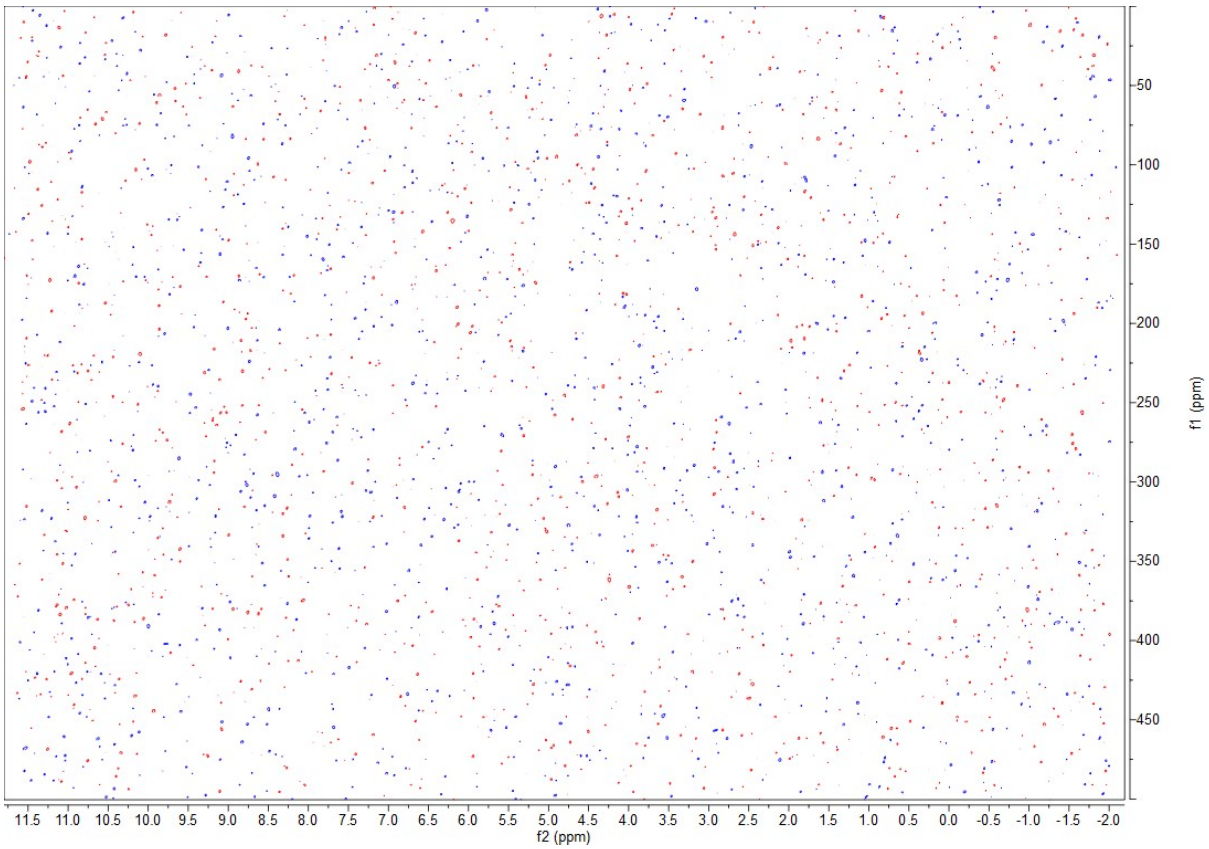


Figure S5. ^{1}H-^{15}N HMBC NMR spectrum of untreated PHW using the same concentrating factor as HSQC. The S/N ratio is too low to acquire useful information.

Table S1. Characteristics of PHW derived from food waste HTL processing

Characteristic	Value
pH	7.97
Conductivity	18.4 mS cm^{-1}
COD	57,500 ± 200 mg L^{-1}
DOC	17,853 ± 287 mg L^{-1}
IC	404 ± 12 mg L^{-1}
TN	2,812 ± 101 mg L^{-1}
NO3--N	87.6 ± 6.2 mg L^{-1}
NH3-N	1,248 ± 6 mg L^{-1}
ORG-N	1,476 ± 89 mg L^{-1}
Xylitol	411 ± 12 mg L^{-1}
Glycolate	190 ± 8 mg L^{-1}
Glycerol	4,992 ± 253 mg L^{-1}
Acetate	4,319 ± 6 mg L^{-1}
1,3-PDO	1,247 ± 17 mg L^{-1}
Propionate	1,275 ± 26 mg L^{-1}
Ethanol	3,160 ± 23 mg L^{-1}
Butyrate	374 ± 2 mg L^{-1}
Isovalerate	228 ± 9 mg L^{-1}
2-butanone	221 ± 2 mg L^{-1}
p-cresol	86 ± 6

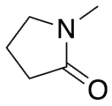
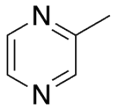
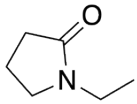
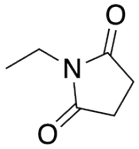
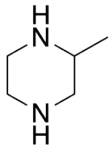
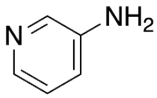
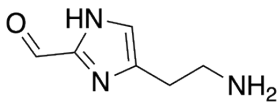
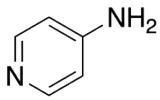
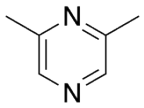
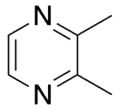
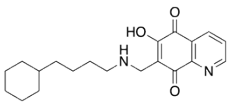
Table S2. HPLC database of common metabolites/salts and their elution time.
Note that the column used is Agilent Hi-Plex H. Different column pressure, flow rate, mobile phase concentration etc. could also alter the elution time.

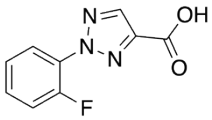
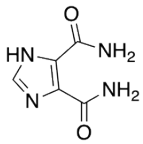
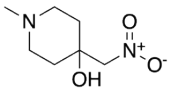
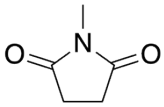
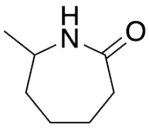
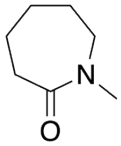
Chemicals	Peak Location (min)
sulfate	7.4-7.5
chloride	7.5
citrate	9.19-9.20
tartrate	9.7
sucrose	9.9-10.0 (and two side peaks at ~ 8.8 and 10.7)
glucose	10.05-10.07
pyruvate	10.2-10.8
galactose	10.6-10.7
xylose	10.69-10.70
fructose	10.72-10.75
mannitol	10.97-10.98
sorbitol	11.1-11.2
arabinose	11.44-11.45
xylitol	11.9-12.0
succinate	12.9-13.0
glycolic acid	13.02-13.04
1,6-anhydro-β-D-glucose	13.0-13.1
lactate	13.55-13.62
glycerol	13.89-13.92
3-hydroxypropionate	14.0-14.1
formate	14.3-14.5

3--hydroxybutyrate	14.58-14.64
fumarate	15.0-15.2
acetate	15.7
ethylene glycol	16.35-16.36
levulinic acid	17.05-17.07
1,2-propanediol	17.50-17.51
1,3-propanediol	17.74-17.75
propionate	18.7
2,3-butanediol	18.7-18.8
methanol	19.10-19.13
1,3-butanediol	19.5-19.8
1,2-butanediol	21.5
isobutyrate	21.8
ethanol	21.97-22.00
acetone	22.60-22.62
butyrate	23.4
isopropanol (2-propanol)	24.79-24.83
2,5-hexanedione	25.0-25.1
isovalerate	27.9
1-propanol	28.3
2-butanone	29.3-29.4
isobutyraldehyde	29.8-29.9
5-HMF	31.9-32.4
valerate	33.4
2-butanol	33.43-33.55

2-methyl-1-propanol	34.8-34.9
3-methyl-2-butanone	35.6-35.8
2-cyclopenten-1-one	37.5-37.8
3-methyl-2(5H)-furanone	38.5-38.8
3-pentanone	39.0-39.3
2-pentanone	39.2-39.5
1-butanol	39.63-39.82
benzoate	40.0-40.6
furfural	47.6-48.2
m-cresol	81.4-91.4
p-cresol	92.7-96.7

Table S3. Heterocyclic compounds in PHW identified through GC-MS

compound name	Structure	Formula	MW (g/mol)	CAS #
1-Methyl-2-pyrrolidinone		C_5H_9NO	99.13	872-50-4
2-Methylpyrazine		$C_5H_6N_2$	94.11	109-08-0
1-Ethyl-2-pyrrolidinone		$C_6H_{11}NO$	113.16	2687-91-4
1-Ethyl-2,5-pyrrolidinedione		$C_6H_9NO_2$	127.14	2314-78-5
2-Methylpiperazine		$C_5H_{12}N_2$	100.16	109-07-9
3-Aminopyridine		$C_5H_6N_2$	94.11	462-08-8
2-Formylhistamine		$C_6H_9N_3O$	139.16	/
4-Aminopyridine		$C_5H_6N_2$	94.11	504-24-5
2,6-Dimethylpyrazine		$C_6H_8N_2$	108.14	108-50-9
2,3-Dimethylpyrazine		$C_6H_8N_2$	108.14	108-50-9
Quinoline-5,8-dione-6-ol, 7-[[(4-cyclohexylbutyl)amino]methyl]-		$C_{20}H_{26}N_2O_3$	342.40	/

2-(2-Fluorophenyl)-2H-1,2,3-triazole-4-carboxylic acid		$C_9H_6FN_3O_2$	207.16	51306-44-6
Imidazole-4,5-dicarboxamide		$C_5H_6N_4O_2$	154.13	83-39-6
1-Methyl-4-(nitromethyl)piperidin-4-ol		$C_7H_{14}N_2O_3$	174.20	/
1-methylpyrrolidine-2,5-dione		$C_5H_7NO_2$	113.11	1121-07-9
7-Methylazepan-2-one		$C_7H_{13}NO$	127.18	1985-48-4
1-Methylcaprolactam		$C_7H_{13}NO$	127.18	2556-73-2