Advanced treatment of hydrothermal liquefaction wastewater with nanofiltration to recover carboxylic acids

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Supplementary

Table S1 Mass balance during NF of acidic or as-is model HTL-WW-01 solution.

	Mass	Conductivity	DOC	DOC
	g	mS/cm	mg/L	mg
Feed	200.8	1.44	5019	1007.8
Permeate	60.5	1.22	4153	252.3
Retentate	140.4	1.52	5239	735.6
Mass Balance (%)	**-0.05**	-	-	**1.98**

Table S2 Mass balance during NF of acidic or as-is model HTL-WW-02 solution.

	Mass	Conductivity	DOC	DOC
	g	mS/cm	mg/L	mg
Feed	201.0	1.45	5535	1112.5
Permeate	60.8	1.27	5126	311.7
Retentate	140.8	1.49	5950	837.8
Mass Balance (%)	**-0.29**	-	-	**-3.32**

Table S3 Mass balance during NF of acidic or as-is model HTL-WW-03 solution.

	Mass	Conductivity	DOC	DOC
	g	mS/cm	mg/L	mg
Feed	200.5	1.45	5433	1089.3
Permeate	60.7	1.25	5046	306.3
Retentate	140.3	1.50	5798	813.5
Mass Balance (%)	**-0.25**	-	-	**-2.80**

Table S4 Mass balance during NF of acidic or as-is model HTL-WW-04 solution.

	Mass	Conductivity	DOC	DOC
	g	mS/cm	mg/L	mg
Feed	201.8	1.19	5718	1153.9
Permeate	60.7	0.95	4974	301.9
Retentate	141.8	1.28	5977	847.5
Mass Balance (%)	**-0.35**	-	-	**0.39**

Table S5 Mass balance during NF of pH 8 model HTL-WW-01 solution.

	Mass	Conductivity	DOC	DOC	Alkalinity [a]	Alkalinity
	g	mS/cm	mg/L	mg	g/L	g
Feed	203.5	9.78	4769	970.5	5.47	1.11
Permeate	62.8	2.23	833	52.3	1.33	0.08
Retentate	140.8	12.06	6154	866.5	7.37	1.04
Mass Balance (%)	**-0.05**	-	-	**5.33**	-	**-0.90**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S6 Mass balance during NF of pH 8 model HTL-WW-02 solution.

	Mass	Conductivity	DOC	DOC	Alkalinity [a]	Alkalinity
	g	mS/cm	mg/L	mg	g/L	g
Feed	204.5	9.60	5421	1108.6	5.85	1.20
Permeate	68.0	1.99	1308	88.9	1.15	0.08
Retentate	135.6	12.96	7117	965.0	7.97	1.08
Mass Balance (%)	**0.44**	-	-	**4.93**	-	**3.33**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S7 Mass balance during NF of pH 8 model HTL-WW-03 solution.

	Mass g	Conductivity mS/cm	DOC mg/L	DOC mg	Alkalinity [a] g/L	Alkalinity g
Feed	204.4	9.46	5288	1080.9	5.75	1.18
Permeate	63.3	2.09	1386	87.7	1.30	0.08
Retentate	141.1	12.11	7130	1006	7.58	1.07
Mass Balance (%)	**0.00**	-	-	**1.19**	-	**2.54**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S8 Mass balance during NF of pH 8 model HTL-WW-04 solution.

	Mass	Conductivity	DOC	DOC	Alkalinity [a]	Alkalinity
	g	mS/cm	mg/L	mg	g/L	g
Feed	204.4	9.31	5229	1068.8	6.14	1.26
Permeate	61.6	2.18	1416	87.2	1.86	0.12
Retentate	142.6	11.99	6819	972.4	8.23	1.17
Mass Balance (%)	**0.10**	-	-	**0.86**	-	**2.38**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S9 Mass balance during NF of pH 9 model HTL-WW-02 solution.

	Mass	Conductivity	DOC	DOC	Alkalinity [a]	Alkalinity
	g	mS/cm	mg/L	mg	g/L	g
Feed	201.2	10.27	5462	1099.0	5.55	1.12
Permeate	63.6	1.70	1237	78.7	0.86	0.06
Retentate	137.2	13.60	7257	995.6	7.76	1.07
Mass Balance (%)	**0.20**	-	-	**2.25**	-	**0.89**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S10 Mass balance during NF of pH 10 model HTL-WW-02 solution.

	Mass	Conductivity	DOC	DOC	Alkalinity [a]	Alkalinity
	g	mS/cm	mg/L	mg	g/L	g
Feed	202.6	10.39	5361	1086.0	5.43	1.10
Permeate	64.9	1.93	1190	77.2	1.00	0.07
Retentate	136.9	13.62	7234	990.3	7.71	1.06
Mass Balance (%)	**0.39**	-	-	**1.70**	-	**-2.73**

[a] Alkalinity (g/L) is defined as the amount of acid required to obtain a methyl orange end-point expressed in terms of acetate

Table S11 Charges on the membrane and the state of solutes in the synthetic HTL-WW solutions.

pH	Membrane charge	Acetic acid	Latic acid	Propionic acid	Isobutyric acid	Phenol	Butanone	Pyridine
		pK_a (4.75)	pK_a (3.86)	pK_a (4.88)	pK_a (4.84)	pK_a (10)		pK_a (5.25)
2.6	+	unionized	unionized	unionized	unionized	unionized	unionized	+
8	-	ionized	ionized	ionized	ionized	unionized	unionized	unionized

Figure Captions

Fig. S1 UV-Vis spectra of raw model HTL-WW solutions separated by the NF90 membrane after dilution 1:100 in DI water: HTL-WW-01 (A); HTL-WW-02 (B); HTL-WW-03 (C); HTL-WW-04 (D).

Fig. S2 UV-Vis spectra of pH 8 model HTL-WW solutions separated by the NF90 membrane after dilution 1:100 in DI water: HTL-WW-01 (A); HTL-WW-02 (B); HTL-WW-03 (C); HTL-WW-04 (D).
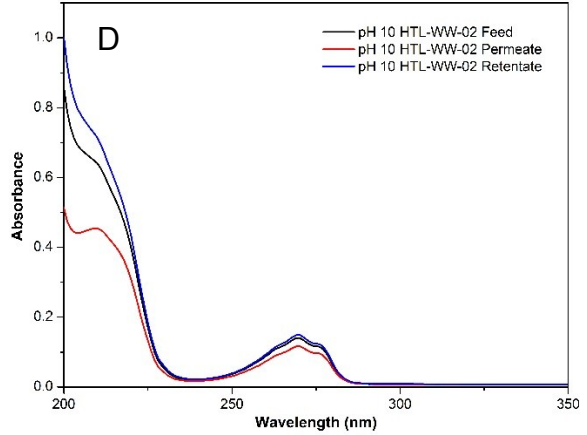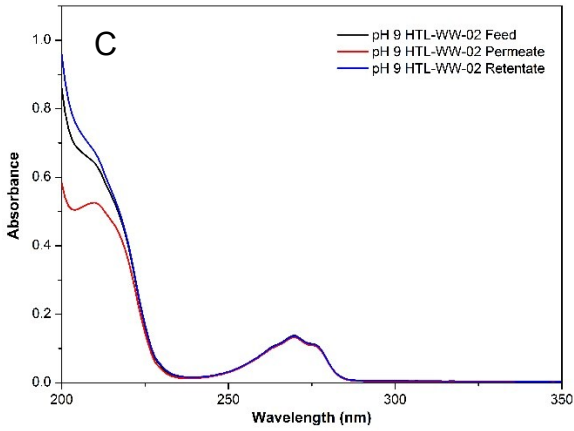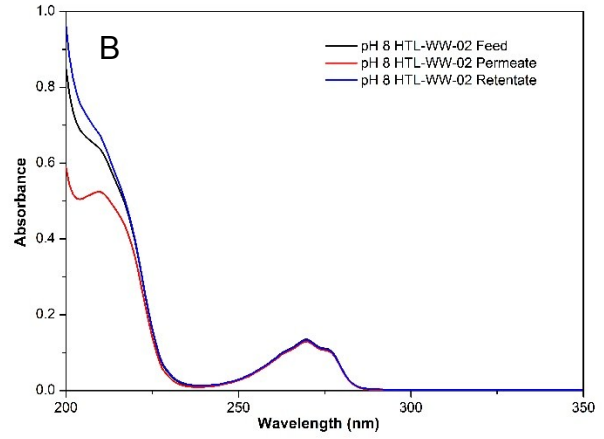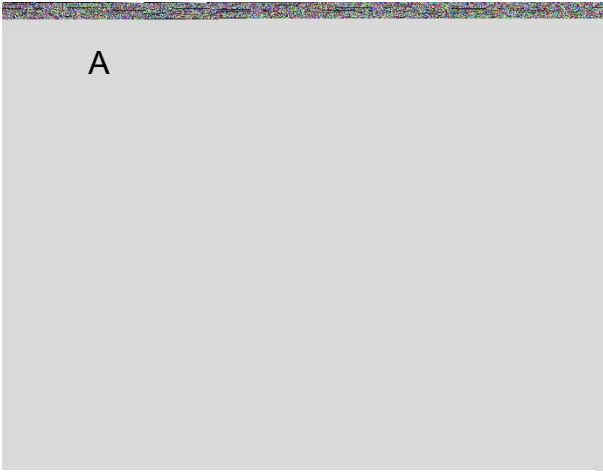

Fig. S3 UV-Vis spectra of HTL-WW-02 solutions separated by the NF90 membrane with respect to pH adjustment after dilution 1:100 in DI water: intial pH (A); pH 8 (B); pH 9 (C); and pH 10 (D).
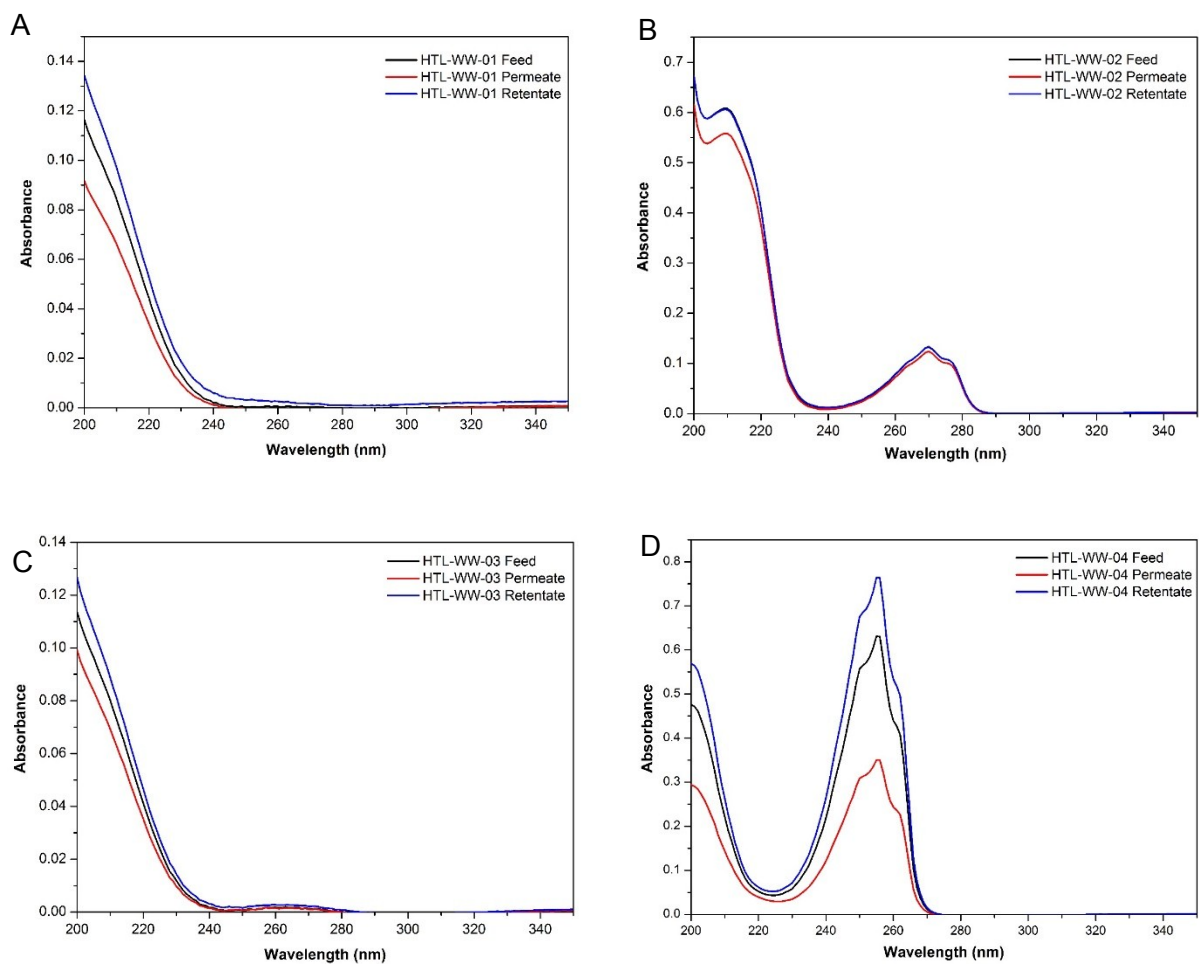
Fig. S1 UV-Vis spectra of raw model HTL-WW solutions (pH ~2.6) separated by the NF90 membrane after dilution 1:100 in DI water: HTL-WW-01 (A); HTL-WW-02 (B); HTL-WW-03 (C); HTL-WW-04 (D).
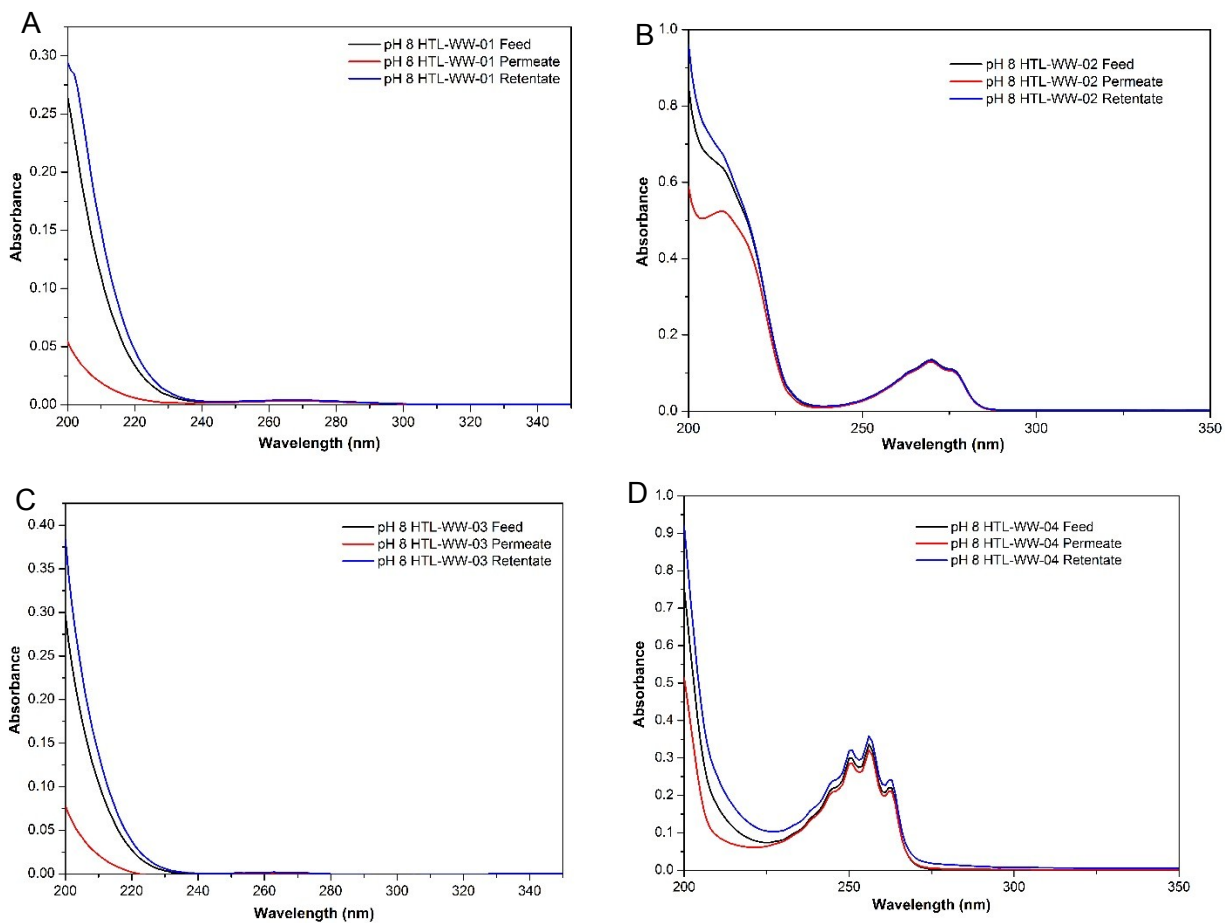
Fig. S2 UV-Vis spectra of pH 8 model HTL-WW solutions separated by the NF90 membrane after dilution 1:100 in DI water: HTL-WW-01 (A); HTL-WW-02 (B); HTL-WW-03 (C); HTL-WW-04 (D).

Fig. S3 UV-Vis spectra of HTL-WW-02 solutions separated by the NF90 membrane with respect to pH adjustment after dilution 1:100 in DI water: intial pH 2.4 (A); pH 8 (B); pH 9 (C); and pH 10 (D).