Electronic Supplementary Information

Sustainable keratin recovery process using a bio-based ionic liquid aqueous solution and its techno-economic assessment

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Table S1. Parameters used to estimate the contribution of a refrigeration system.

Parameters	Value
Electricity ($kW_{electricity} \cdot MJ_{refrigerant}^{-1}$)	0.074
Cooling water ($MJ \cdot MJ_{refrigerant}^{-1}$)	0.74
CO_2 emissions due to electricity generation ($kg \cdot kWh^{-1}$)	0.45
Capital cost per unit of refrigerant ($\$ \cdot MJ_{refrigerant}^{-1}$)	3.10

Table S2. Values used to estimate the utility cost of the keratin recovery process.

Parameters	Value
Fuel ($\$ \cdot MJ^{-1}$)	2.74
Steam ($\$ \cdot kg^{-1}$)	0.12
Cooling water ($\$ \cdot m^{-3}$)	0.055
Electricity ($\$ \cdot kWh^{-1}$)	0.3
Chicken feathers ($\$ \cdot ton^{-1}$)	20

Table S3. Parameters used to estimate the total capital cost.

Parameters	Abbreviation	Equation
Direct field cost	DF	Sum of the installed costs (estimated through Aspen)
Direct field labour cost	DFLC	$0.25 \times DF$
Indirect field cost	IFC	$1.15 \times DFLC$
Total field cost	TFC	$DF + DFLC + IFC$
Home office cost	HOC	$0.3 \times DF$
Other project cost	OPC	$0.03 \times DF + 0.15 \times (TFC + HOC)$
Total project cost	TPC	$TFC + HOC + OPC$

Table S4. Parameters used to estimate the fixed cost.

Parameters	Equation
Maintenance (M)	$0.1 \times \mathrm{TFC}$
Laboratory	$0.2 \times \mathrm{LC}$
Supervision	$0.2 \times (\mathrm{LC} + \mathrm{M})$
Plant overhead	$0.5 \times (\mathrm{LC} + \mathrm{M})$
Depreciation	$0.1 \times \mathrm{TFC}$
Insurance	$0.01 \times \mathrm{TFC}$
Local taxes	$0.02 \times \mathrm{TFC}$
Royalties	$0.01 \times \mathrm{TFC}$

Table S5. Results of RSM for keratin recovery from chicken feathers using an aqueous solution of $[N_{111(2OH)}][C_1CO_2]$.

Assay	Coded values			Response
	X_1	X_2	X_3	Yield (%)
1	-1	-1	-1	50.14
2	1	-1	-1	28.87
3	-1	1	-1	55.89
4	1	1	-1	64.51
5	-1	-1	1	80.01
6	1	-1	1	15.31
7	-1	1	1	90.84
8	1	1	1	24.98
9	-1.68	0	0	64.06
10	1.68	0	0	67.99
11	0	-1.68	0	78.30
12	0	1.68	0	86.79
13	0	0	-1.68	43.23
14	0	0	1.68	93.57
15	0	0	0	80.15
16	0	0	0	83.17
17	0	0	0	82.15

Table S6. Estimated coefficients obtained from the polynomial model and statistical criteria of keratin recovery from chicken feathers.

Parameters	Coefficients	Standard deviation	t-student (4)	P-value	Confidence Limit -90 %	Confidence Limit +90 %
Interception	86.6615	2.6965	32.1388	0.0000	80.9130	92.4100
Ethanol concentration (L) [1]	-10.0117	1.6344	-6.1258	0.0036	-13.4959	-6.5275
Ethanol concentration (Q) [1]	-11.3390	1.6366	-6.9286	0.0022	-14.8279	-7.8501
Time (L) [2]	5.5811	1.6344	3.4149	0.0269	2.0969	9.0653
Time (Q) [2]	-5.4858	1.6366	-3.3521	0.0285	-8.9747	-1.9970
Solution:coagulant ratio (L) [3]	7.0577	1.6344	4.3184	0.0124	3.5735	10.5419
Solution:coagulant ratio (Q)	-10.4975	1.6366	-6.4144	0.0030	-13.9864	-7.0086
Ethanol concentration x solution:coagulant ratio	-14.7388	2.1344	-6.9052	0.0023	-19.2891	-10.1884

Table S7. ANOVA data for keratin recovery from chicken feathers using bio-based IL obtained from RSM.

Factors	Sum of squares	Degree of freedom	Mean Square	F-value	P-value
Ethanol concentration (L) [1]	1367.67	1	1367.67	37.5252	0.0036
Ethanol concentration (Q) [1]	1749.64	1	1749.64	48.0053	0.0022
Time (L) [2]	425.02	1	425.02	11.6614	0.0269
Time (Q) [2]	409.53	1	409.53	11.2363	0.0285
Solution:coagulant ratio (L) [3]	679.67	1	679.67	18.6482	0.0124
Solution:coagulant ratio (Q) [3]	1499.59	1	1499.59	41.1446	0.0030
Solid-liquid ratio x concentration	1737.85	1	1737.85	47.6817	0.0023
Lack or Fit	3469.42	7	495.63	13.5987	0.0119
Pure Error	145.79	4	36.45	-	-

Table S8. Technoeconomic results from the process simulation.

Parameters	Abbreviation	Value
Direct field cost	DF	3.5 m$
Total field cost	TFC	5.4 m$
Total project cost	TPC	7.5 m$
Total annual fixed cost	-	4.5 m$·year^{-1}
Total annual variable cost	-	2.2 m$·year^{-1}
Minimum selling price for keratin	-	22 $·kg^{-1}
CO_2 emissions	-	4.04 $kg_{CO2}·kg_{keratin}^{-1}$

Eq. S1. $\text{Yield (\%)} = 86.66 - 10.01(X_1) - 11.33(X_1^2) + 5.88(X_2) - 5.48(X_2^2) + 7.05(X_3) - 10.50(X_3^2) - 14.73(X_1 \times X_3)$

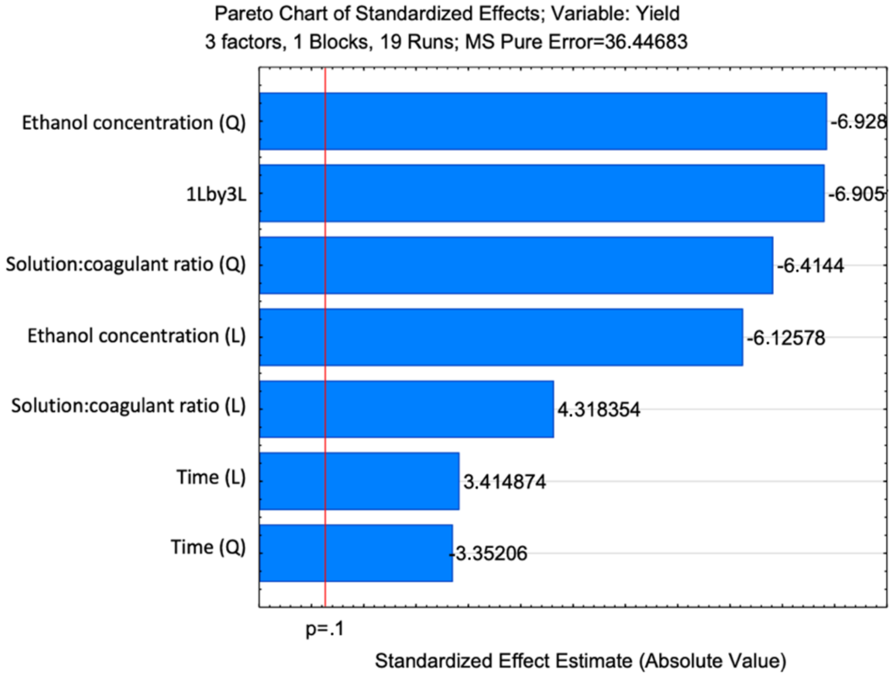

Fig. S1. Pareto diagram for the effects of process parameters on keratin recovery from chicken feathers.

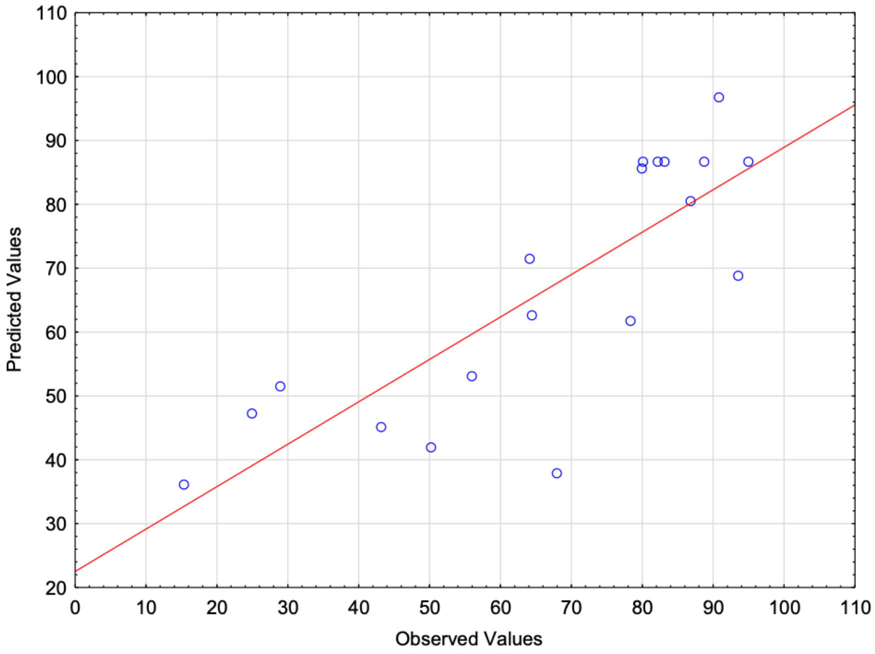

Fig. S2. Predicted and observed values obtained from RSM design.

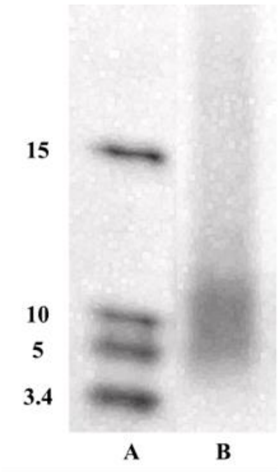

Fig. S3. SDS-PAGE of protein marker (A) and keratin recovered using the optimal conditions (20.25 wt % of ethanol concentration, 5 h, and solution:coagulant ratio of 1:1.45).

<u>Cholinium acetate fresh:</u>

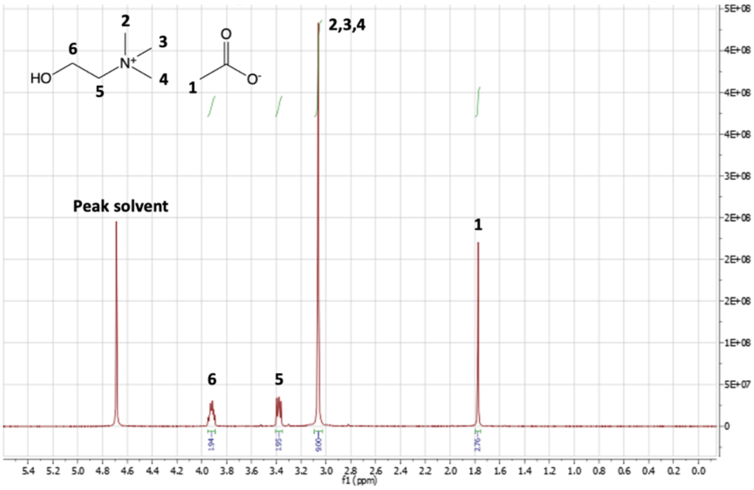

Fig. S4. ^{1}H NMR (D_2O, 300 MHz, [ppm]): 3.922 (2H, m); 3.379 (2H, t, J= 10.2 Hz); 3.062 (3H, s); 1.774 (3H, s).

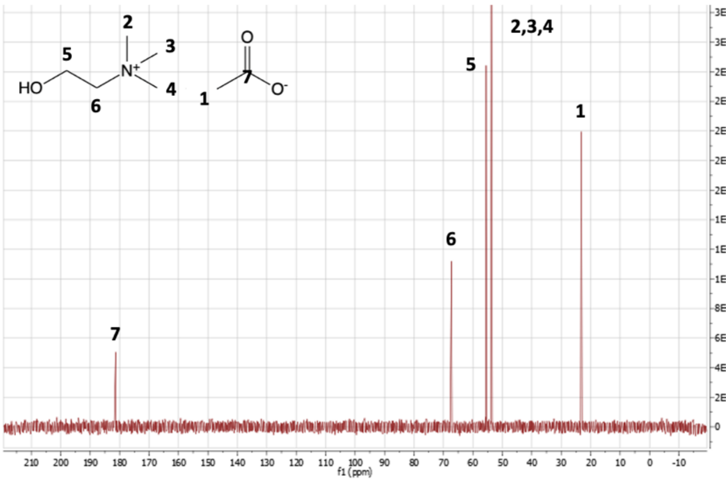

Fig. S5. ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 181.556; 67.563; 55.499; 53.811; 23.065.

Cholinium acetate recovered:

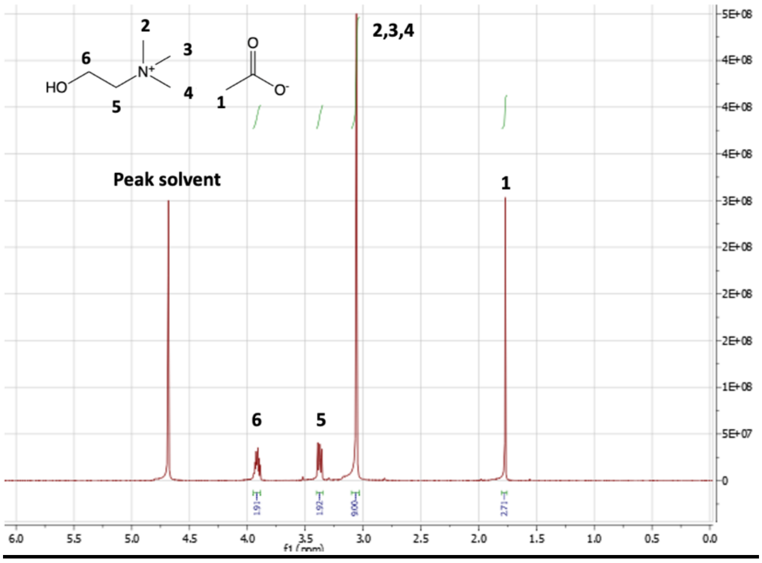

Fig. S6. ^{1}H NMR (D_2O, 300 MHz, [ppm]): 3.908 (2H, m); 3.373 (2H, t, J= 9.9 Hz); 3.057 (3H, s); 1.769 (3H, s).

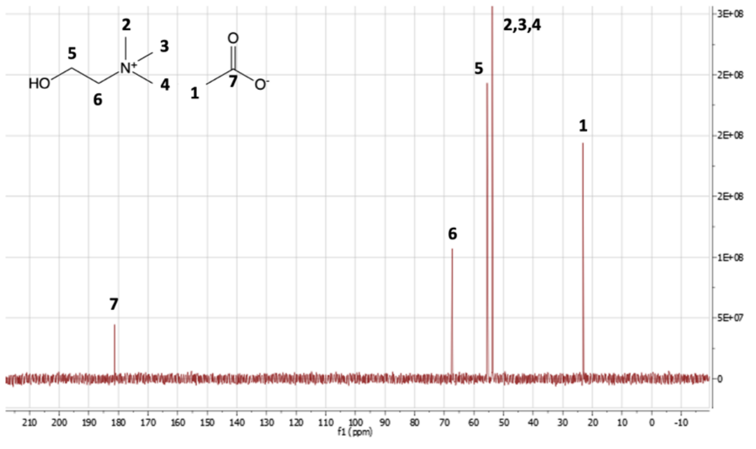

Fig. S7. ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 181.185; 67.271; 55.496; 53.806; 23.089.

References

[1] A. Al-Ghatta, J. D. E. T. Wilton-Ely and J. P. Hallett, From sugars to FDCA: a techno-economic assessment using a design concept based on solvent selection and carbon dioxide emissions, Green Chemistry, 2021, 23, 1716–1733.

[2] A. R. Abouelela, A. Al-Ghatta, P. Verdía, M. Shan Koo, J. Lemus and J. P. Hallett, Evaluating the Role of Water as a Cosolvent and an Antisolvent in [HSO4]-Based Protic Ionic Liquid Pretreatment, ACS Sustainable Chemistry & Engineering, 2021, 9, 10524–10536.