Supplementary Information

for

Green process for separation and recovery of 5-hydroxymethylfurfural from carboxylic acid-choline chloride deep eutectic solvents

Table of contents

1. Influences of different extraction conditions on the extraction of 5-HMF

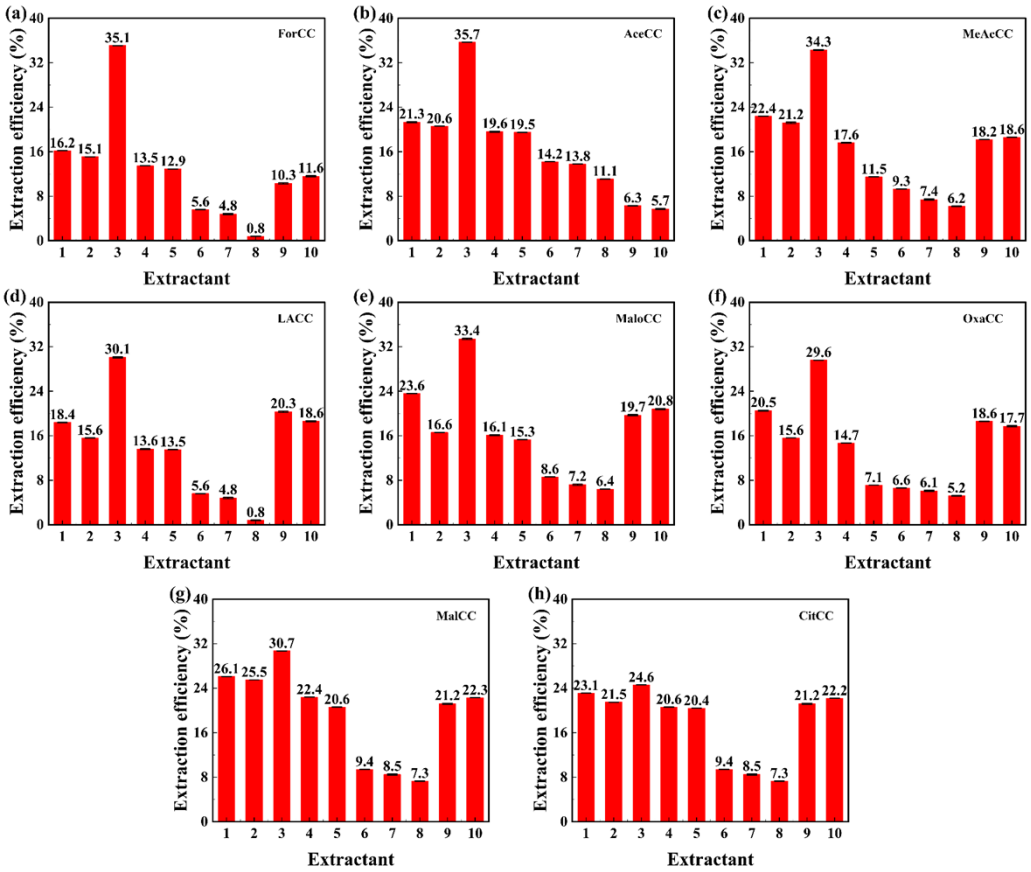

Fig. S1 The extraction efficiencies of different organic solvents for the extraction of 5-HMF.

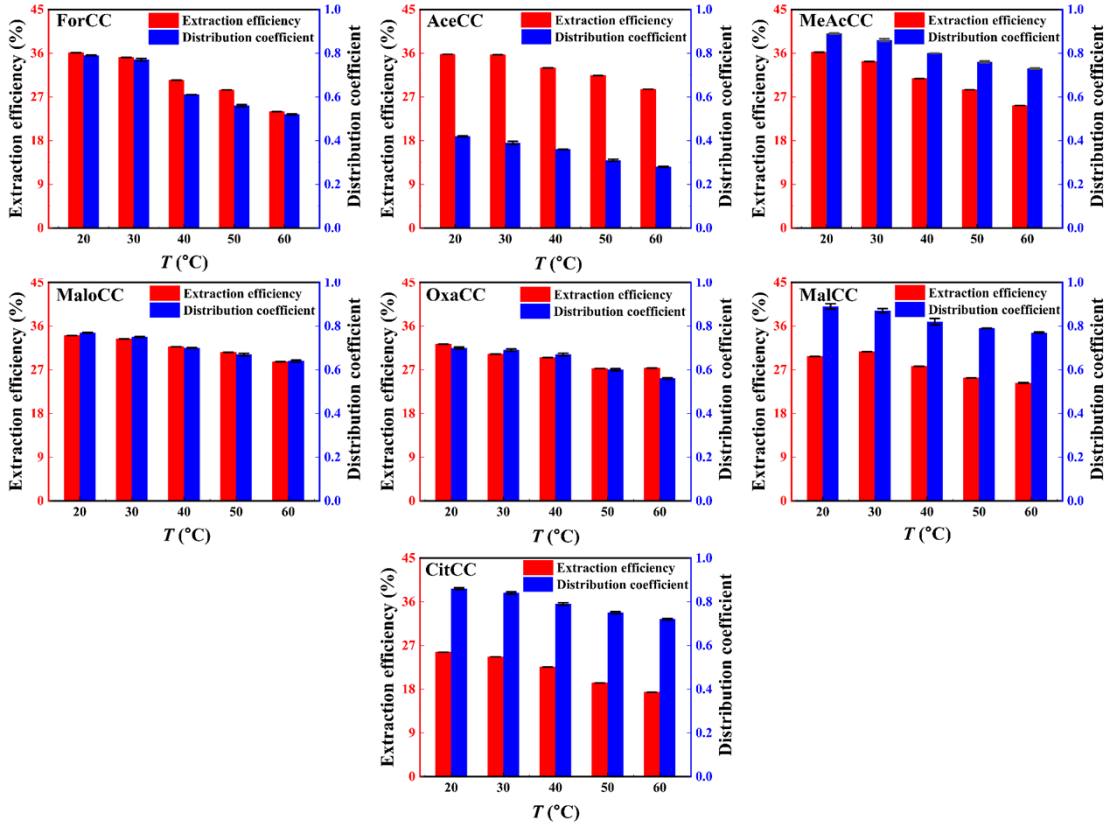

Fig. S2 The effect of temperature on the extraction of 5-HMF by THF in different DESs.

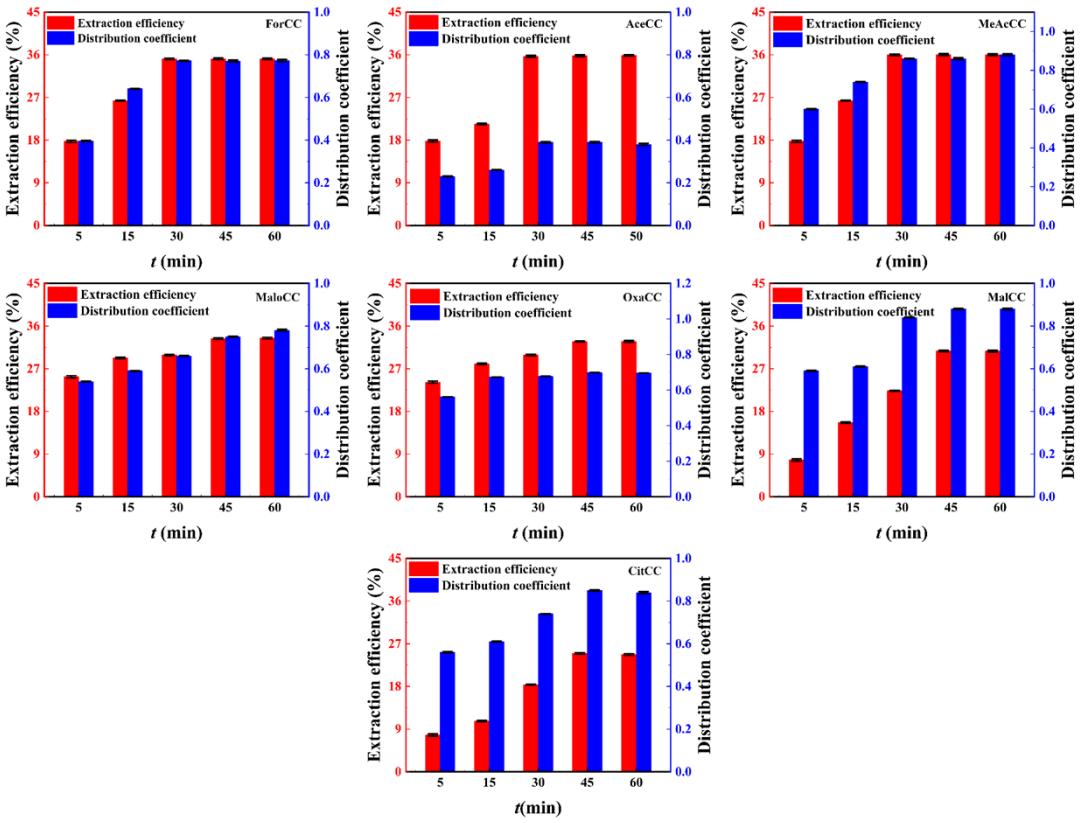

Fig. S3 The effect of time on the extraction of 5-HMF by THF in different DESs.

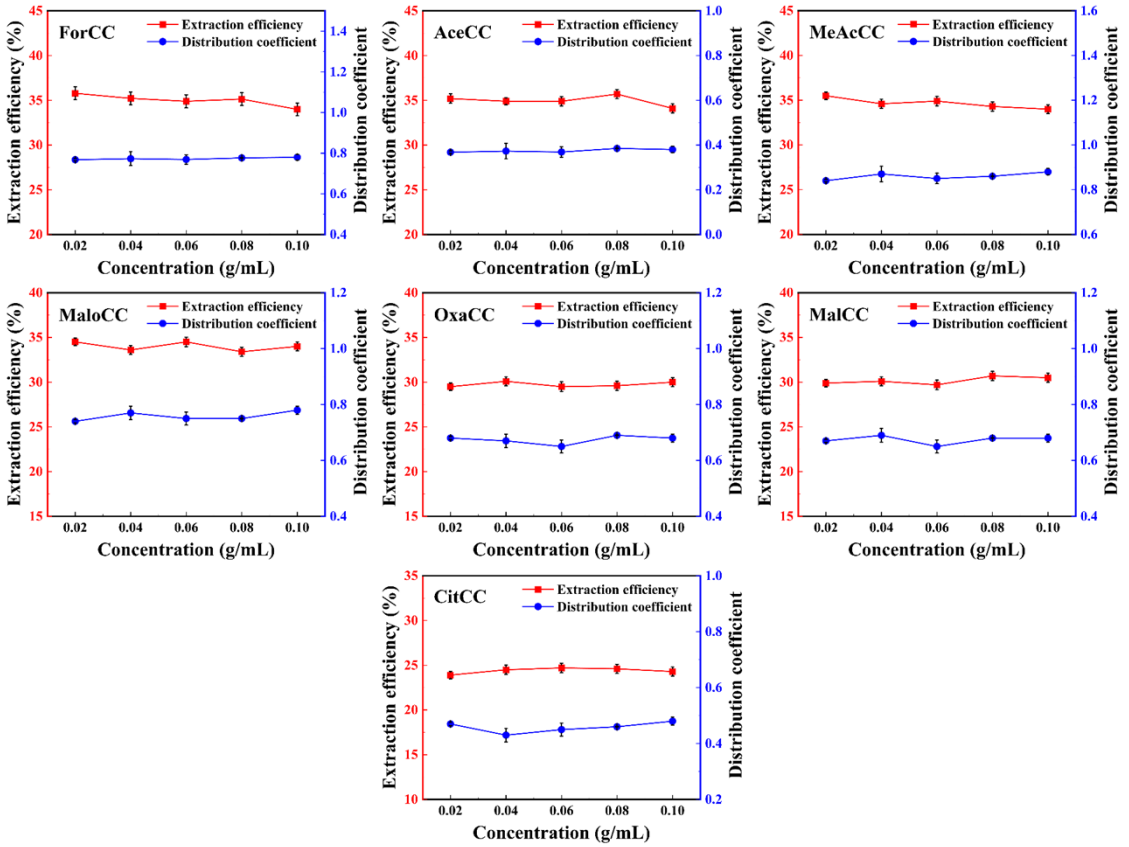

Fig. S4 The effect of concentration on the extraction of 5-HMF by THF in different DESs.

2. Standard curves

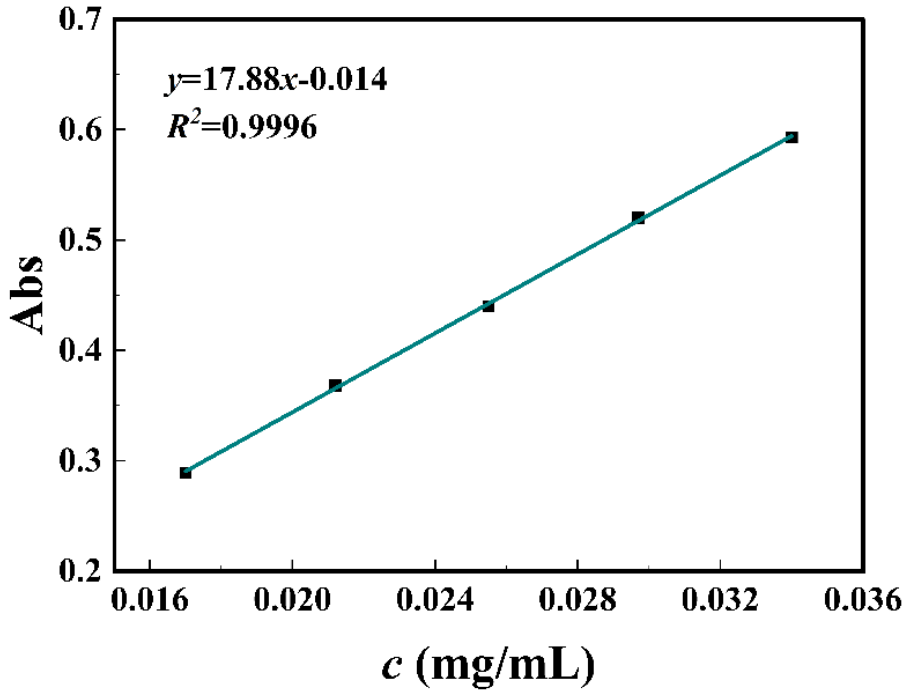

Fig. S5 The standard curve of D-fructose concentration.

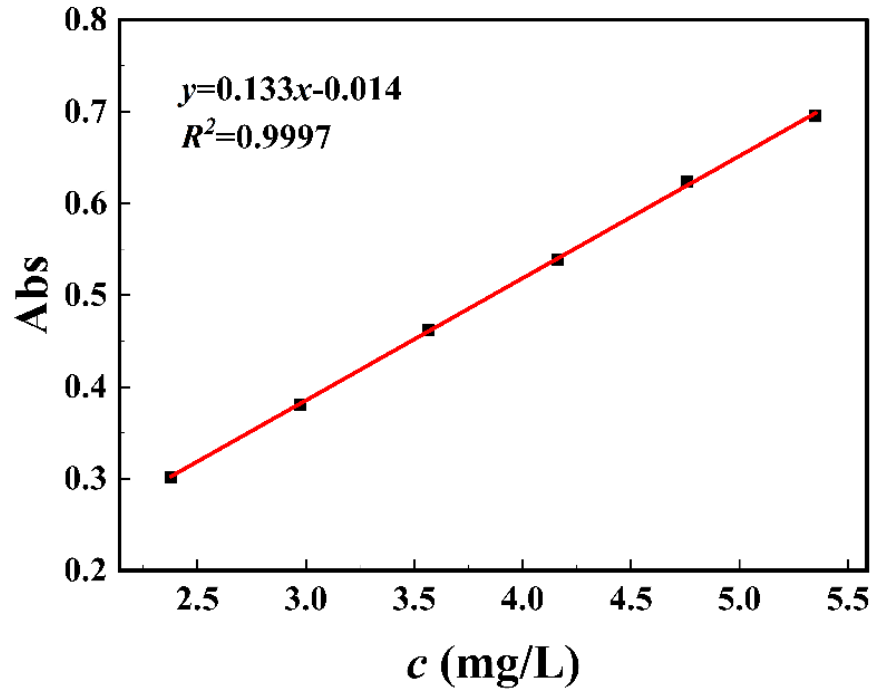

Fig. S6 The standard curve of 5-HMF concentration.

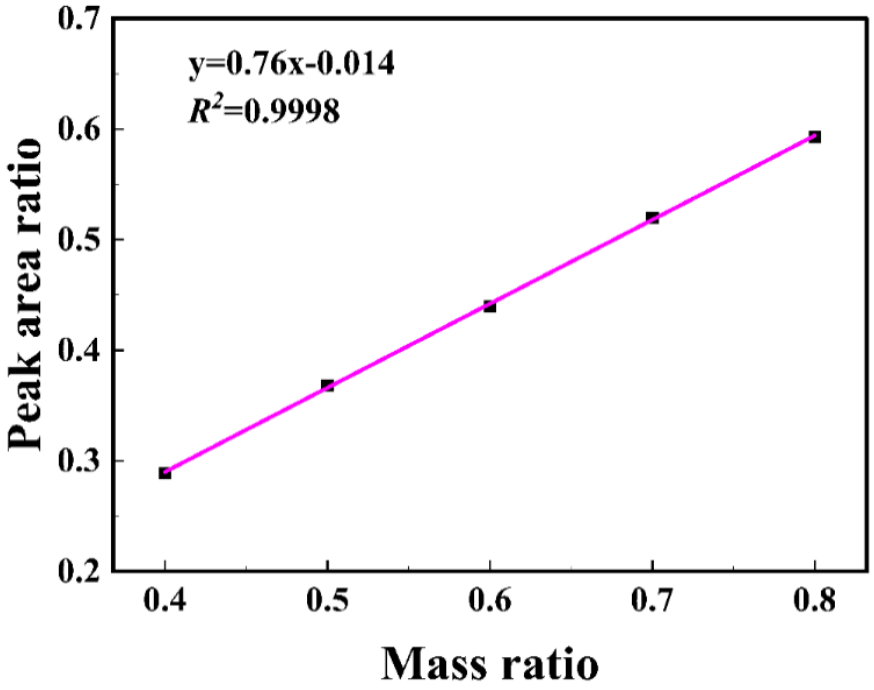

Fig. S7. The standard curve of THF concentration.

3. Relevant tables

Table S1. The reaction conditions for the conversion of fructose to 5-HMF in different solvents reported in the literature.

Reaction solvent	Fructose mass ratio (%)	*T* (°C)	Yield (%)	$c_{5\text{-HMF}}$(g/mL)	Ref.
Imidazole: benzene sulfonic acid	10	100	90.1	0.06	1
ChCl: lactic acid	33.3	140	87.2	0.24	2
ChCl: p-toluene sulfonic acid	2.5	80	90.7	0.02	3
ChCl: Fructose	20	120	72	0.10	4
ChCl: N, N'-tetramethylurea	50	110	89	0.06	5
ChCl: Phenol	15-20	110	67	0.07~0.09	6
ChCl: Citric acid	5	120	91.03	0.03	7
ChCl: Fructose	25	100	90.3	0.12	8

Table S2. The polarity of the common organic solvents.

Organic solvents	Polarity
Acetone	5.4
Dioxane	4.8
Tetrahydrofuran	4.2
Ethyl acetate	4.3
Methyl isobutyl ketone	4.2
Methylene chloride	3.4
Ethyl ether	2.9
Toluene	2.4
2-Methylfuran	3.6
2-Methyltetrahydrofuran	3.2

Table S3. The distribution coefficients for the extraction of 5-HMF by different extractants in DESs at 30 °C.

DES / Extractant	ForCC	AceCC	MeAcCC	LACC	MaloCC	OxaCC	MalCC	CitCC
Acetone	0.52	0.22	0.77	0.37	0.65	0.48	0.86	0.76
Dioxane	0.46	0.21	0.67	0.36	0.53	0.47	0.84	0.54
THF	0.77	0.39	0.86	0.59	0.75	0.69	0.87	0.84
EtOAc	0.41	0.18	0.62	0.34	0.32	0.42	0.51	0.52
MIBK	0.37	0.18	0.59	0.31	0.32	0.36	0.36	0.51
MeCh	0.11	0.16	0.39	0.11	0.28	0.28	0.35	0.35
Ethyl ether	0.12	0.16	0.37	0.12	0.22	0.16	0.31	0.31
Toluene	0.01	0.12	0.36	0.01	0.11	0.11	0.23	0.23
2-MeF	0.32	0.16	0.46	0.39	0.39	0.56	0.41	0.41
2-MeTHF	0.33	0.16	0.56	0.38	0.42	0.42	0.43	0.43

Notes: MeCh is methylene chloride; 2-MeF is 2-methylfuran; 2-MeTHF is 2-methyltetrahydrofuran.

Table S4. The distribution coefficients for the extraction of 5-HMF at different temperatures.

T (°C) / DES	20	30	40	50	60
ForCC	0.79	0.77	0.61	0.56	0.52
AceCC	0.42	0.39	0.36	0.31	0.28
MeAcCC	0.89	0.86	0.80	0.76	0.73
LACC	0.63	0.59	0.55	0.53	0.51
MaloCC	0.77	0.75	0.70	0.67	0.64
OxaCC	0.70	0.69	0.67	0.60	0.56
MalCC	0.89	0.87	0.82	0.79	0.77
CitCC	0.86	0.84	0.79	0.75	0.72

Table S5. The distribution coefficients for the extraction of 5-HMF at different concentrations.

c (g/mL) / DES	0.02	0.04	0.06	0.08	0.10
ForCC	0.77	0.78	0.77	0.78	0.79
AceCC	0.37	0.37	0.37	0.39	0.38
MeAcCC	0.84	0.87	0.85	0.86	0.88
LACC	0.59	0.60	0.59	0.59	0.58
MaloCC	0.74	0.77	0.75	0.75	0.78
OxaCC	0.68	0.67	0.65	0.69	0.68
MalCC	0.87	0.89	0.85	0.88	0.88
CitCC	0.86	0.84	0.85	0.85	0.84

Table S6. The distribution coefficients for the extraction of 5-HMF at different times.

t (min) / DES	5	15	30	45	60
ForCC	0.40	0.64	0.77	0.78	0.79
AceCC	0.23	0.26	0.39	0.39	0.38
MeAcCC	0.60	0.74	0.86	0.86	0.88
LACC	0.44	0.46	0.54	0.59	0.58
MaloCC	0.54	0.59	0.66	0.75	0.78
OxaCC	0.56	0.62	0.63	0.69	0.68
MalCC	0.59	0.61	0.84	0.88	0.88
CitCC	0.56	0.61	0.74	0.85	0.84

Table S7. The distribution coefficients for the extraction of 5-HMF with different inorganic salts.

Inorganic salt	No adding	NaCl	K_2SO_4	KCl	Na_2SO_4
Distribution coefficient	0.59	1.30	1.02	1.14	1.59

Table S8. The distribution coefficients for the extraction of 5-HMF with different concentrations of NaCl solution.

Concentration (mol/L)	0.5	1.0	1.5	2.0
Distribution coefficient	1.05	1.30	1.06	1.00

4. References

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