Support Information

Exploration of benign deep eutectic solvent–water systems for the highly efficient production of furfurylamine from sugarcane bagasse *via* chemoenzymatic cascade catalysis

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Figure Captions

Fig. S1. Image of recombinant plamid.

Fig. S2. The Circular Dichroism (CD) Spectra of KPB-treated (a), [ChCl][EG]–water-treated (b) and [ChCl][Gly]–water-treated ω-transaminase proteins (c); Tm values of KPB-treated (blank), [ChCl][EG]–water-treated and [ChCl][Gly]–water-treated ω-transaminase proteins (d). [Protein samples were treated for 30 min in KPB (100 mM, pH 7.5) or DES–water (20:80, v:v; pH 8.0). KPB-treated and DES-water-treated ω-transaminase proteins (0.10 mg/L) in 20 mM KPB (pH 7.5) were recorded from 180–260 nm (0.1 cm path length) at 20–80 ℃].

Fig. S3. Themostability of ω-transaminase in pRSFDuet-CV-AlaDH cells in KPB (200 mM, pH 8.0), [ChCl][Gly]–water (pH 8.0) and [ChCl][EG]–water (200 mM, pH 8.0) at 35 ℃ (a) and 50 ℃ (b). [The pRSFDuet-CV-AlaDH cells were treated for 0-4 h in KPB (200 mM, pH 8.0), [ChCl][Gly]–water (pH 8.0) and [ChCl][EG]–water (200 mM, pH 8.0) at 35 ℃ (a) and 50 ℃ (b), and then the cells were washed twice with KPB (200 mM, pH 8.0) for the determination of ω-transaminase activity in KPB (200 mM, pH 8.0)]

Fig. S4. Biotransamination of 100 mM FAL into FLA in KPB, DES [ChCl][EG]–water or DES [ChCl][EG]–water at 35 ºC and pH 8.0 (a); Effects of FAL loading (25–125 mM) on the biotransformation of FAL into FLA in KPB (200 mM, pH 8.0) (b), [ChCl][EG]–water (20:80, v:v) (c), and [ChCl][Gly]–water (20:80, v:v) (d).

Fig. S5. HPLC images of standards (FAL, FOL, and FLA), FLA liquor obtained from the biotransamination of 100 mM FAL in KPB (200 mM, pH 8.0), and FLA liquor obtained from the biotransamination of 100 mM FAL in [ChCl][EG]–water (20:80, v:v).

Fig. S6. Different amine donor *L*-alanine (*L*-Ala) (10.0 mol *L*-Ala/mol FAL), isopropylamine (IPA) (3.0 mol IPA/mol FAL) and NH_4Cl (2.0 mol NH_4Cl/mol FAL) on the biotranamination of 50-100 mM FAL into FLA at 35 ^oC and pH 8.0 [ChCl][EG]–water (20:80, v:v).

Fig. S7. Chemical and chemoenzymatic routes for the transamination of FAL into FLA.

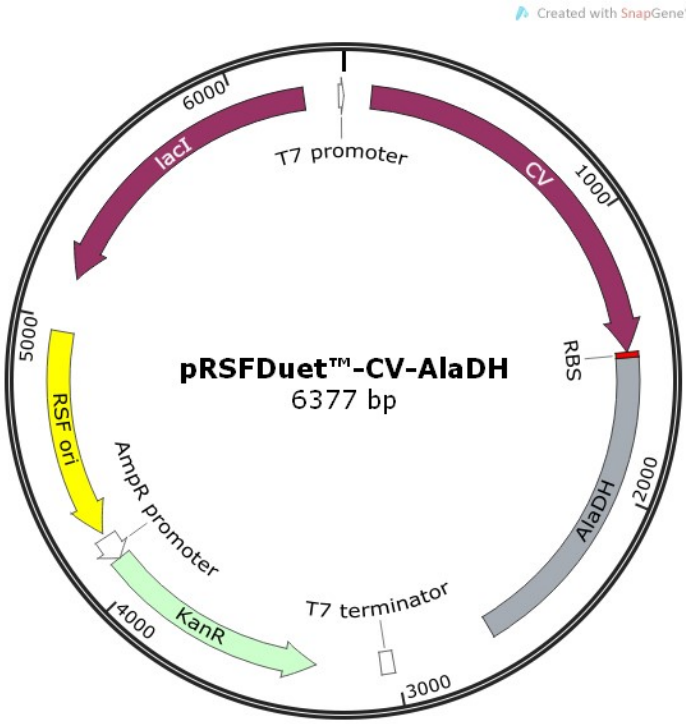
Created with SnapGene®
pRSFDuet™-CV-AlaDH
6377 bp
6000
1000
2000
3000
4000
5000
lacI
T7 promoter
CV
RBS
AlaDH
T7 terminator
KanR
AmpR promoter
RSF ori

Fig. S1

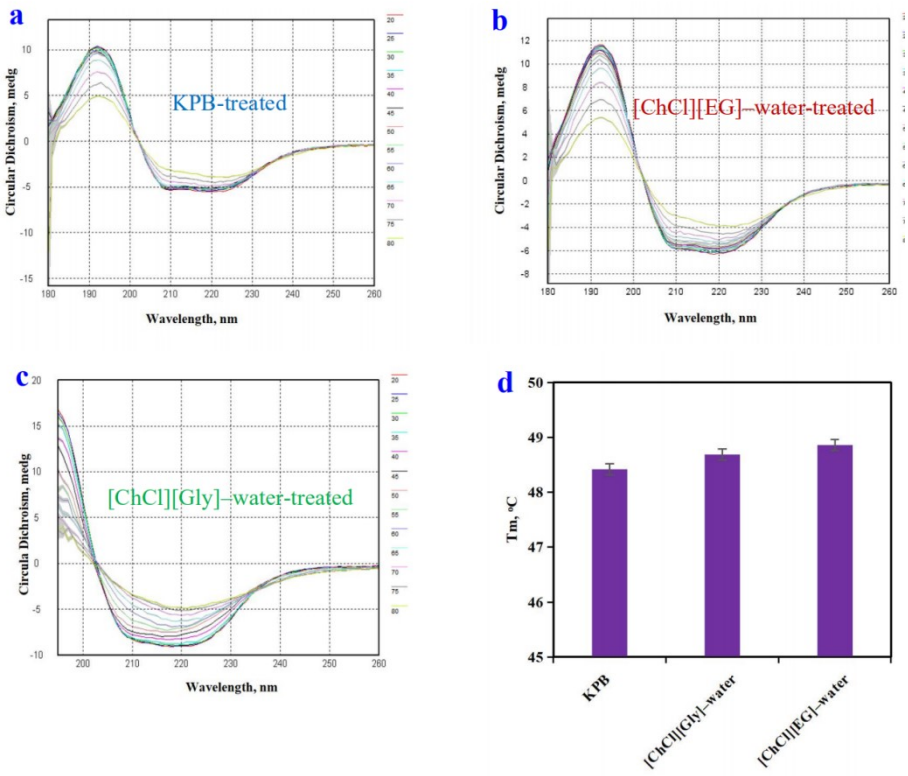
a
KPB-treated
Circular Dichroism, medg
Wavelength, nm
b
[ChCl][EG]–water-treated
Circular Dichroism, medg
Wavelength, nm
c
[ChCl][Gly]–water-treated
Circula Dichroism, medg
Wavelength, nm
d
Tm, °C
KPB
[ChCl][Gly]-water
[ChCl][EG]-water

Fig. S2

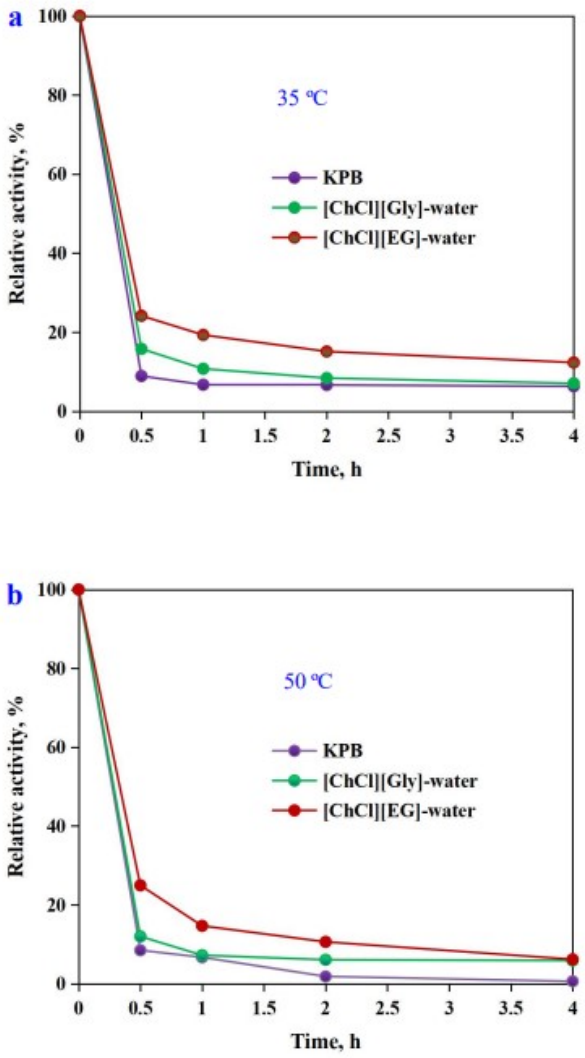
a
100
80
60
40
20
0
Relative activity, %
35 ℃
KPB
[ChCl][Gly]-water
[ChCl][EG]-water
0
0.5
1
1.5
2
2.5
3
3.5
4
Time, h
b
100
80
60
40
20
0
Relative activity, %
50 ℃
KPB
[ChCl][Gly]-water
[ChCl][EG]-water
0
0.5
1
1.5
2
2.5
3
3.5
4
Time, h

Fig. S3

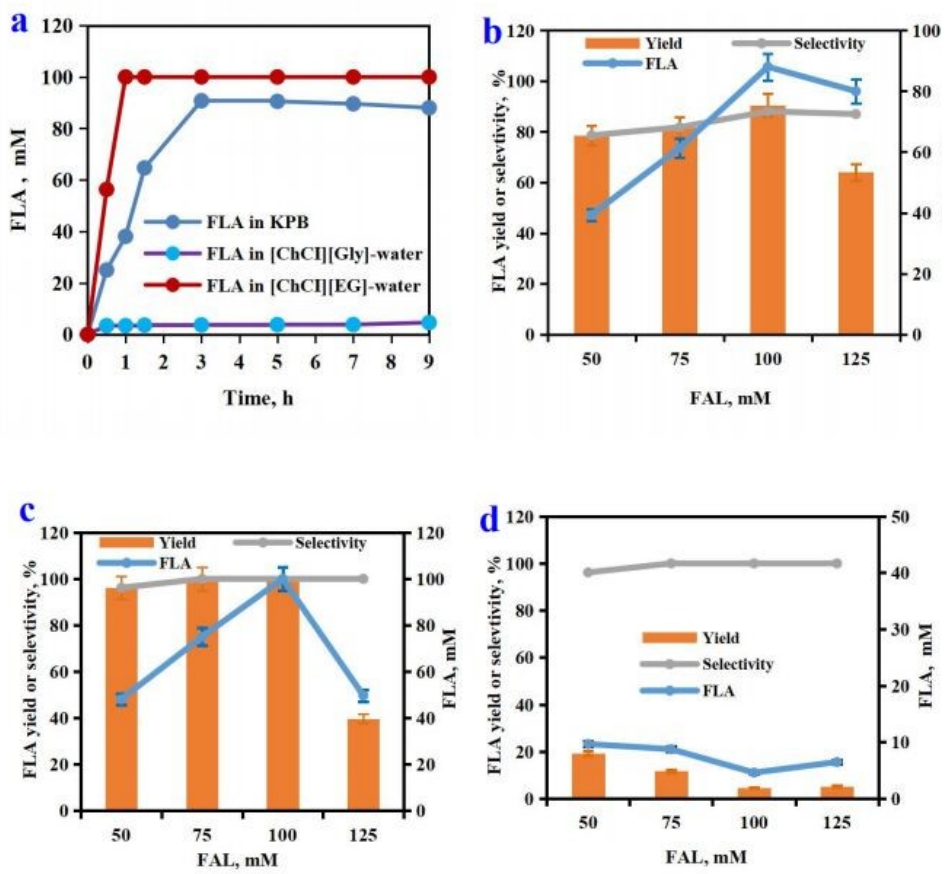
a
FLA , mM
Time, h
FLA in KPB
FLA in [ChCl][Gly]-water
FLA in [ChCl][EG]-water
b
FLA yield or selevtivity, %
FAL, mM
Yield
Selectivity
FLA
c
FLA yield or selevtivity, %
FLA, mM
FAL, mM
Yield
Selectivity
FLA
d
FLA yield or selevtivity, %
FLA, mM
FAL, mM
Yield
Selectivity
FLA

Fig. S4

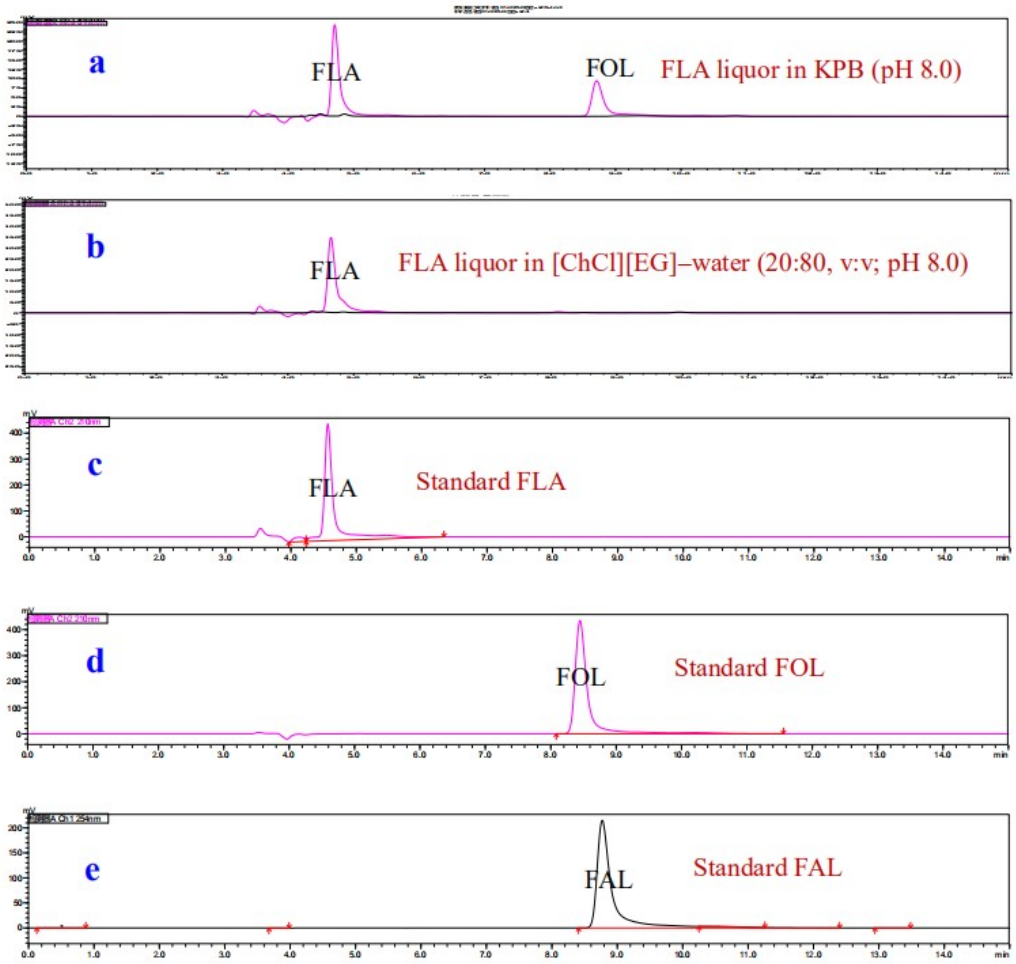
a
FLA
FOL
FLA liquor in KPB (pH 8.0)
b
FLA
FLA liquor in [ChCl][EG]–water (20:80, v:v; pH 8.0)
c
FLA
Standard FLA
d
FOL
Standard FOL
e
FAL
Standard FAL

Fig. S5

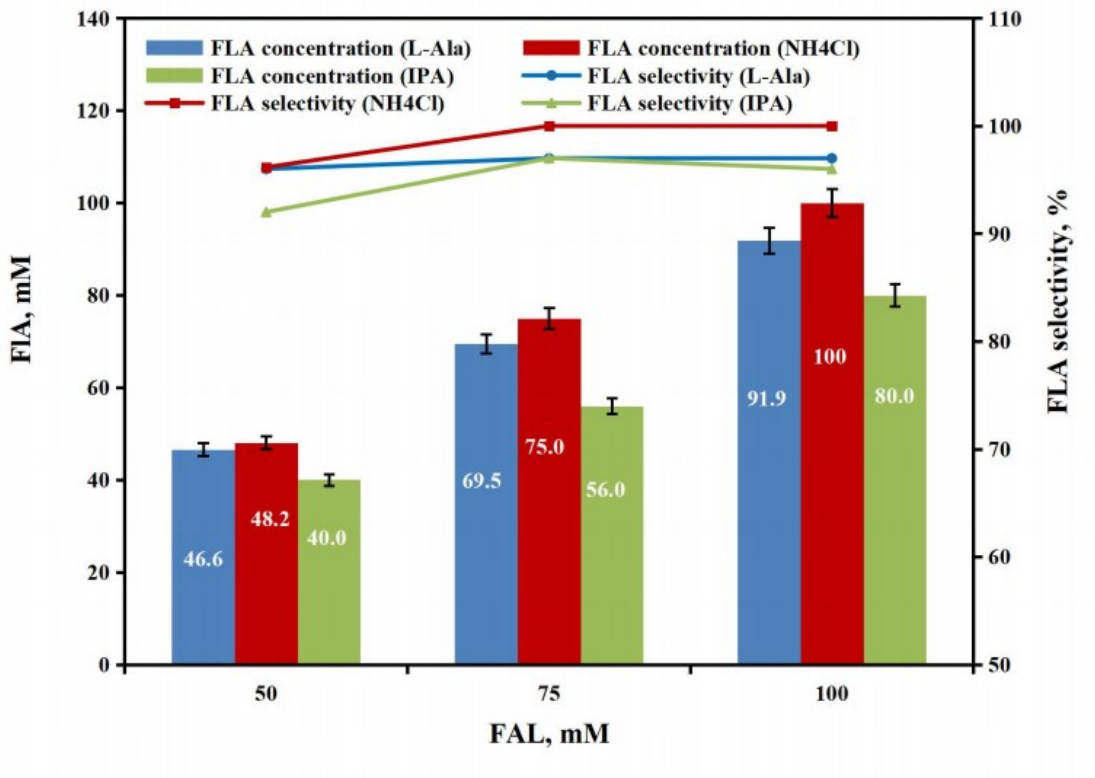
FLA concentration (L-Ala)
FLA concentration (NH4Cl)
FLA concentration (IPA)
FLA selectivity (L-Ala)
FLA selectivity (NH4Cl)
FLA selectivity (IPA)
FlA, mM
FLA selectivity, %
FAL, mM
46.6
48.2
40.0
69.5
75.0
56.0
91.9
100
80.0
50
75
100

Fig. S6

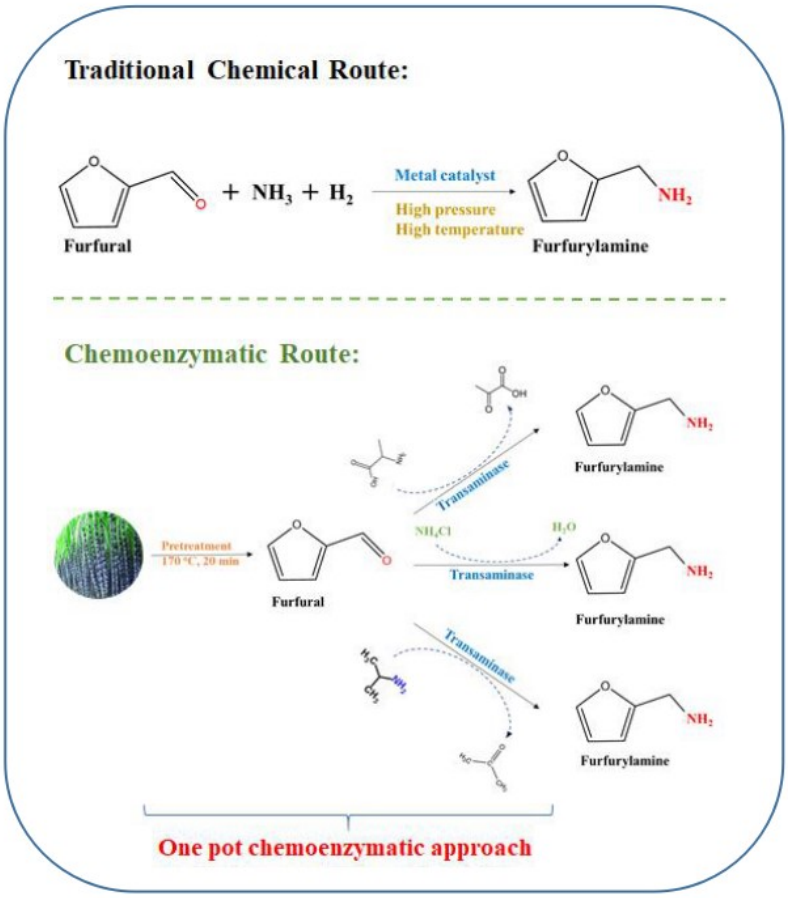
Traditional Chemical Route:
Furfural
+ NH3 + H2
Metal catalyst
High pressure
High temperature
Furfurylamine
Chemoenzymatic Route:
Pretreatment
170 °C, 20 min
Furfural
Transaminase
NH4Cl
H2O
Transaminase
Furfurylamine
Transaminase
Furfurylamine
Furfurylamine
One pot chemoenzymatic approach

Fig. S7