

Electronic Supplementary Material (ESI) for Green Chemistry

Electronic supplementary information

Selective Separation of Lactic, Malic, and Tartaric acids Based on Hydrophobic Deep Eutectic Solvents of Terpenes and Amides

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Content:

Number of pages: **8**

Number of figures: **11**

Number of tables: **7**



Figure S1 Appearance of synthetic hydrophobic DESs of different compositions in this work at ambient temperature.

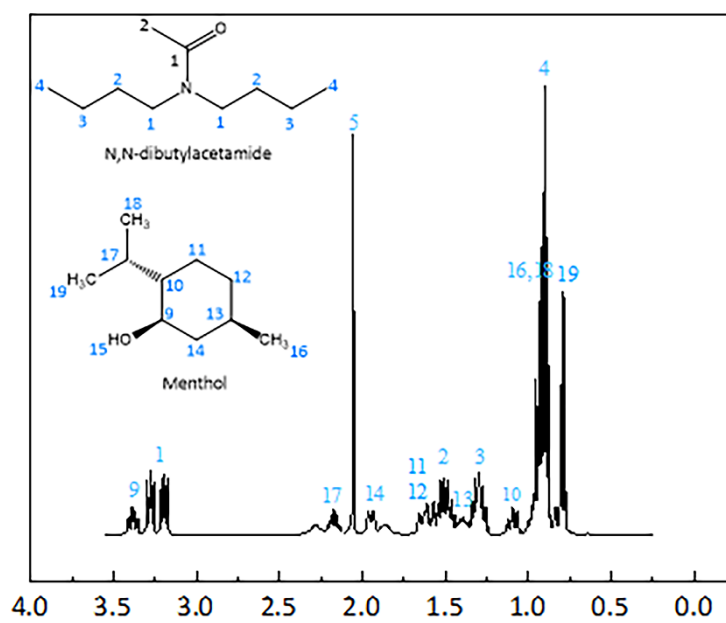


Figure S2 ¹H NMR spectra of deep eutectic solvent DBA : Men 1:1 in CDCl₃. The structure and numbering of both compounds is also depicted.

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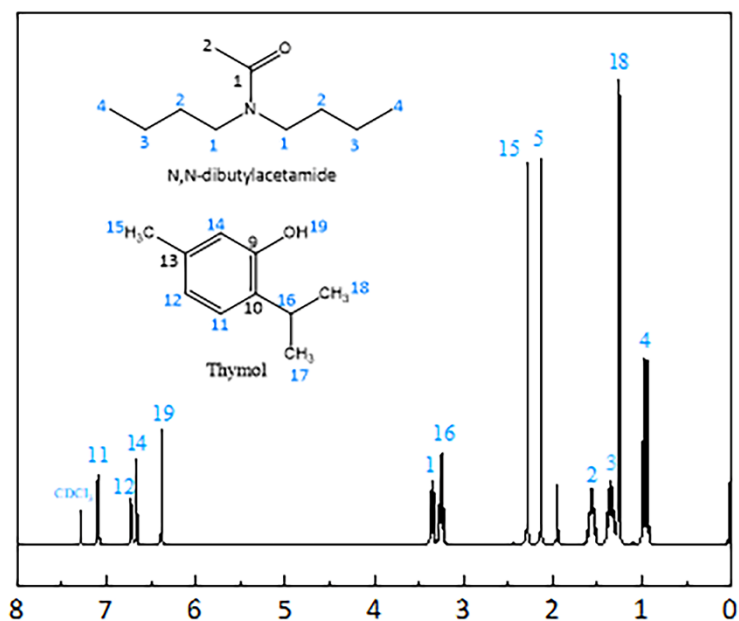


Figure S3 ^1H NMR spectra of deep eutectic solvent DBA : Thy 1:1 in CDCl_3 . The structure and numbering of both compounds is also depicted.

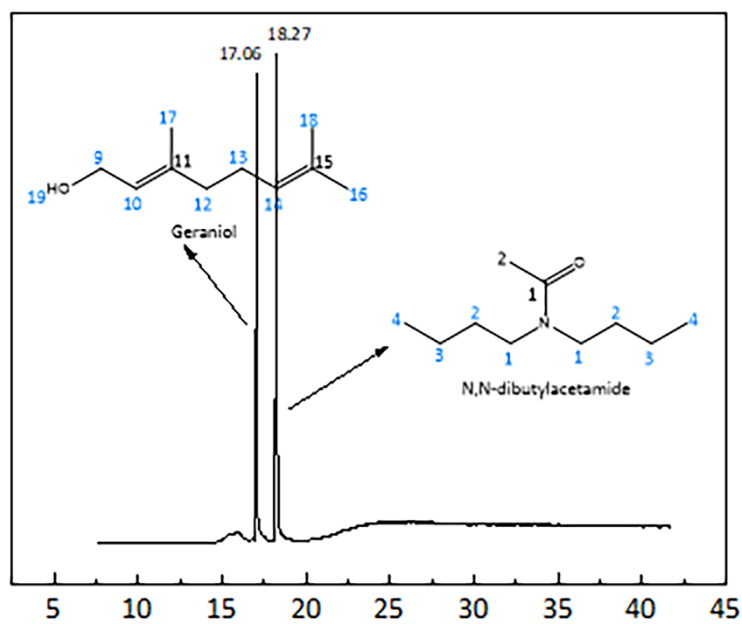


Figure S4 The total ions chromatogram of deep eutectic solvent DBA : Ger 1:1 in $\text{CH}_3\text{CH}_2\text{OH}$

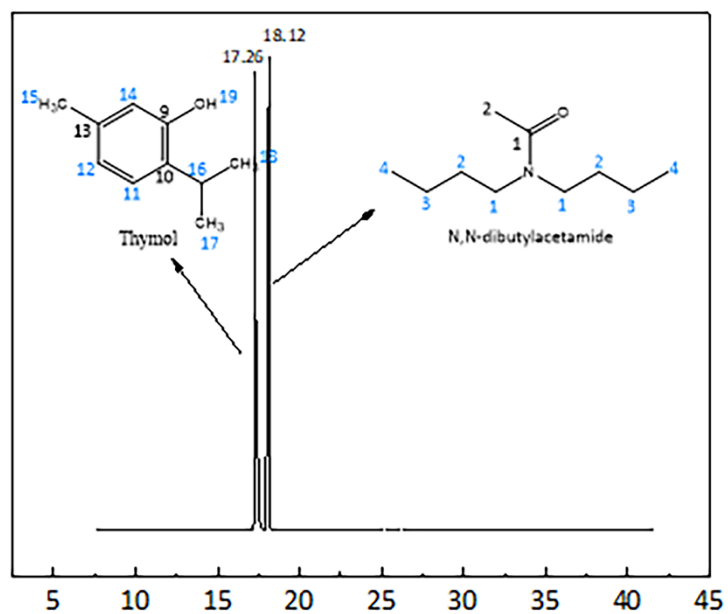


Figure S5 The total ions chromatogram of deep eutectic solvent DBA : Thy 1:1 in $\text{CH}_3\text{CH}_2\text{OH}$

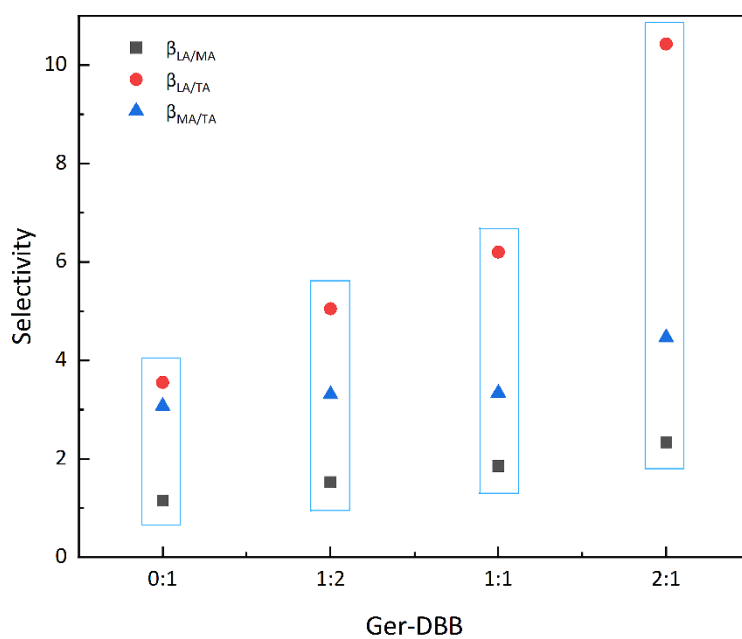


Figure S6 Selectivity (β) in various DES/water systems for , malic acid, tartaric acid, DES/water volume ratio was 1, Ger-DBB at different mole ratio.

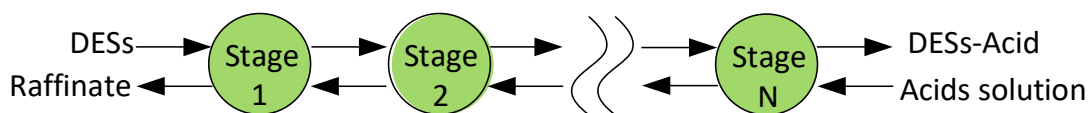


Figure S7 Countercurrent extraction flow chart

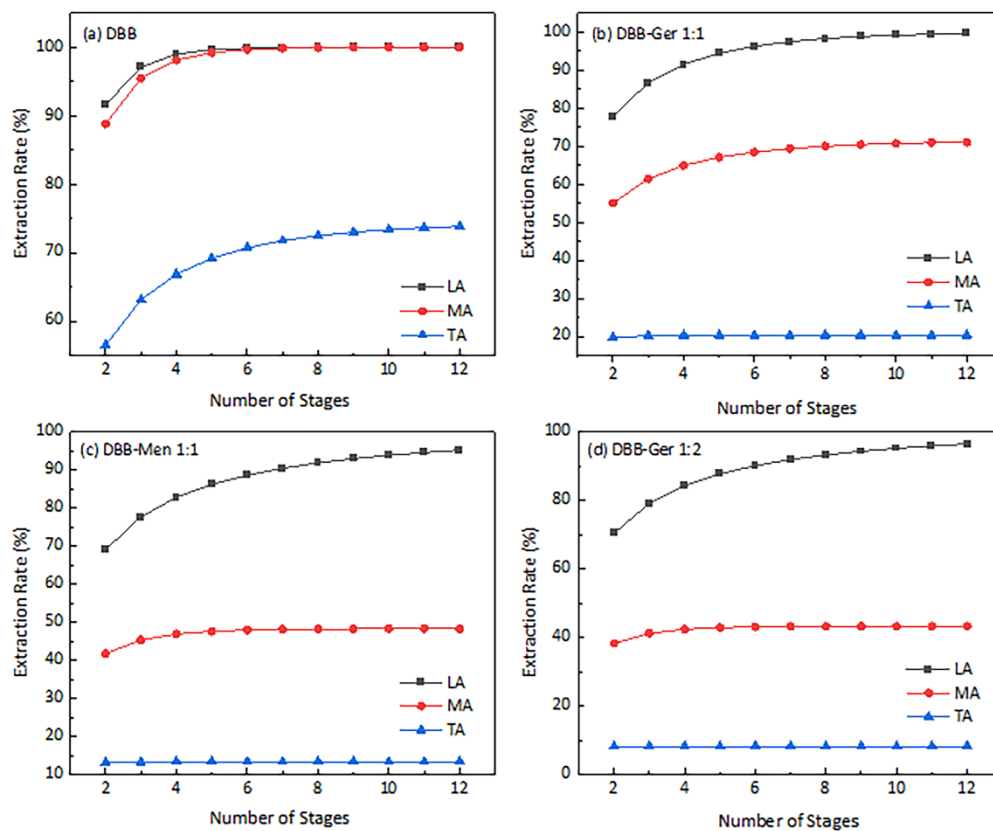


Figure S8 Extraction yields in the selective separation of LA, MA, and TA in the simulation of the counter-current extractor with the Kremser method V/L ratio in volume of 1.0. (a) DBB; (b) DBB-Ger mole ratio of 1:1; (c) DBB-Men mole ratio of 1:1; (d) DBB-Ger mole ratio of 1:2

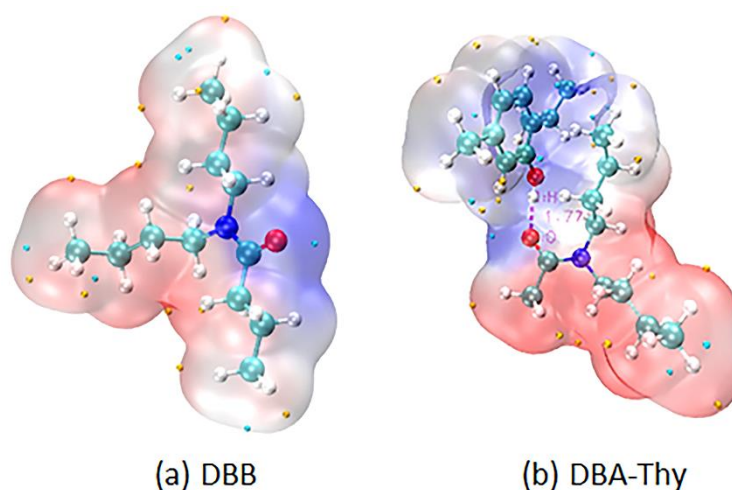


Figure S9 DESS (DBA-Thy) electrostatic potential values mapped on van der Waals surface. Minima and maxima of the ESP on the vdW surface are drawn as cyan and orange, respectively. (negative regions are indicated in blue, and positive regions are indicated in red).

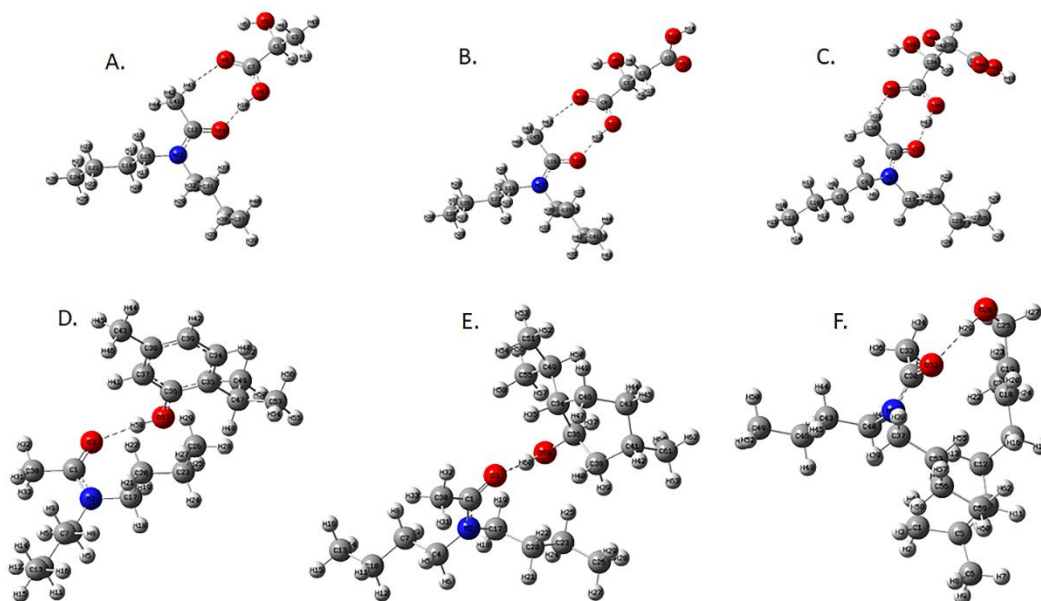


Figure S10 Models of complexes interaction sites optimized at B3LYP/6-31++G(d, p) level.

A.DBA-LA; B. DBA-MA; C. DBA-TA; D. DBA-Ger; E. DBA-Men; F. DBA-Thy.

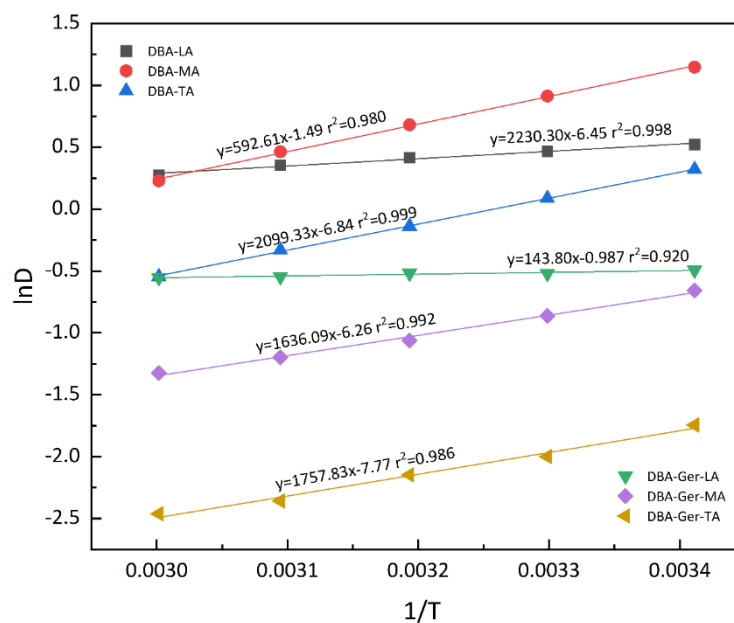


Figure S11 the relationship between lnD and 1/T

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Table S1 Chemical structures of the DESs studied in this work as well as the abbreviation and respective molar mass

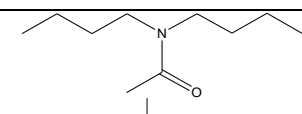
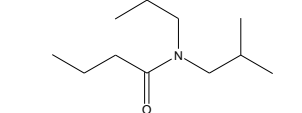
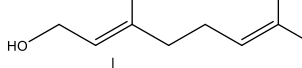
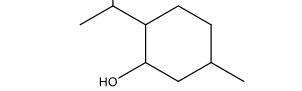
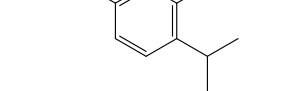
Chemical	Molecular formula	Abbreviation	M	BHBAs structure
N, N-Di-n-butyl-acetamide	C ₁₀ H ₂₁ NO	DBA	171	
N, N-Di-n-butyl-butyramide	C ₁₂ H ₂₅ NO	DBB	199	
geraniol	C ₁₀ H ₁₈ O	Ger	154.14	
menthol	C ₁₀ H ₂₀ O	Men	156.27	
thymol	C ₁₀ H ₁₄ O	Thy	150.22	

Table S2 Equilibrium distribution coefficients (D) in various DES/water systems for lactic acid (LA), malic acid (MA), tartaric acid (TA), DES/water volume ratio was 1, HBA-HBD mole ratio of 1:1.

	D _(LA)	D _(MA)	D _(TA)
DBA-Ger	0.55898	0.40378	0.14472
DBA-Men	0.45263	0.30825	0.10014
DBA-Thy	0.07406	0.01934	0.00572
DBB-Ger	0.35028	0.17301	0.04977
DBB-Men	0.26916	0.12071	0.03331
DBB-Thy	0.04356	0.00616	6.32511E-4

Table S3 Equilibrium distribution coefficients (D) in various DES/water systems for lactic acid (LA), malic acid (MA), tartaric acid (TA) at different mole ratio of DBA-Ger, DES/water volume ratio was 1.

DBA-GER	D _(LA)	D _(MA)	D _(TA)
0:1	1.67831	2.48933	1.07478
1:2	0.8629	0.82785	0.31438
1:1	0.58299	0.41626	0.12146
2:1	0.38392	0.20225	0.04237
1:0	0.1683	0.02399	-0.01804

Table S4 Equilibrium distribution coefficients (D) in various DES/water systems for lactic acid (LA), malic acid (MA), tartaric acid (TA) at different mole ratio of DBB-Ger, DES/water volume ratio was 1.

DBB-GER	D _(LA)	D _(MA)	D _(TA)
0:1	0.70836	0.5896	0.18601
1:2	0.45659	0.27709	0.0763
1:1	0.35968	0.17857	0.05076
2:1	0.28087	0.10813	0.02049
1:0	0.16702	0.02932	-0.00932

Table S5 Selectivity (β) in various DES/water systems for lactic acid, malic acid, tartaric acid, DES/water volume ratio was 1, DBA-HBD mole ratio of 1:1.

	$\beta_{LA/MA}$	$\beta_{LA/TA}$	$\beta_{MA/TA}$
DBA	0.62183	1.37689	2.21425
DBA-Ger	1.38436	3.86253	2.79012
DBA-Men	1.46839	4.51997	3.07818
DBA-Thy	3.82958	12.94391	3.37998

Table S6 Selectivity (β) in various DES/water systems for lactic acid, malic acid, tartaric acid, at different mole ratio of DBA-Ger, DES/water volume ratio was 1.

DBA	$\beta_{LA/MA}$	$\beta_{LA/TA}$	$\beta_{MA/TA}$
0:1	0.62183	1.37689	2.21425
1:2	0.94558	2.35302	2.48845
1:1	1.25919	3.51306	2.78993
2:1	1.69128	5.19903	3.07401

Table S7 Selectivity (β) in various DES/water systems for lactic acid, malic acid, tartaric acid, at different mole ratio of DBB-Ger, DES/water volume ratio was 1.

DBB	$\beta_{LA/MA}$	$\beta_{LA/TA}$	$\beta_{MA/TA}$
0:1	1.15533	3.55503	3.07706
1:2	1.52498	5.0498	3.31139
1:1	1.85627	6.20304	3.34166
2:1	2.33388	10.42894	4.4685