Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

"Supporting Information"

Assessment of Natural-based Chiral Deep Eutectic Solvents Properties for Chiral Drugs Separation: Insights from Molecular Dynamics Simulation

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Figures:

Figure S1. The snapshot of simulation boxes of a) DES1consisting of 300 acetic acid (orange), 150 R-menthol (purple), 150 S-menthol(green), b) DES2 consisting of 200 lauric acid (yellow), 200 R-menthol, 200 S-menthol, and c) DES3 consisting of 400 pyruvic acid (blue), 100 R-menthol, 100 S-menthol.

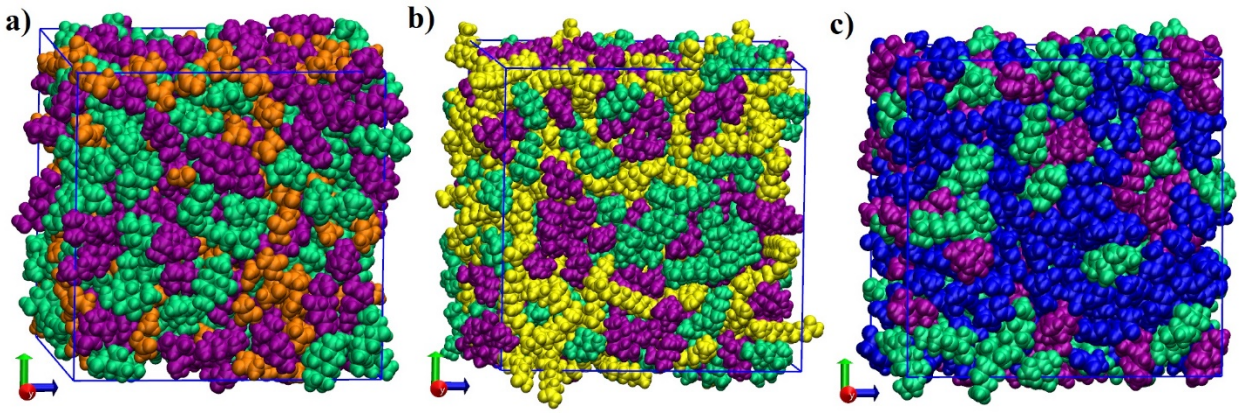
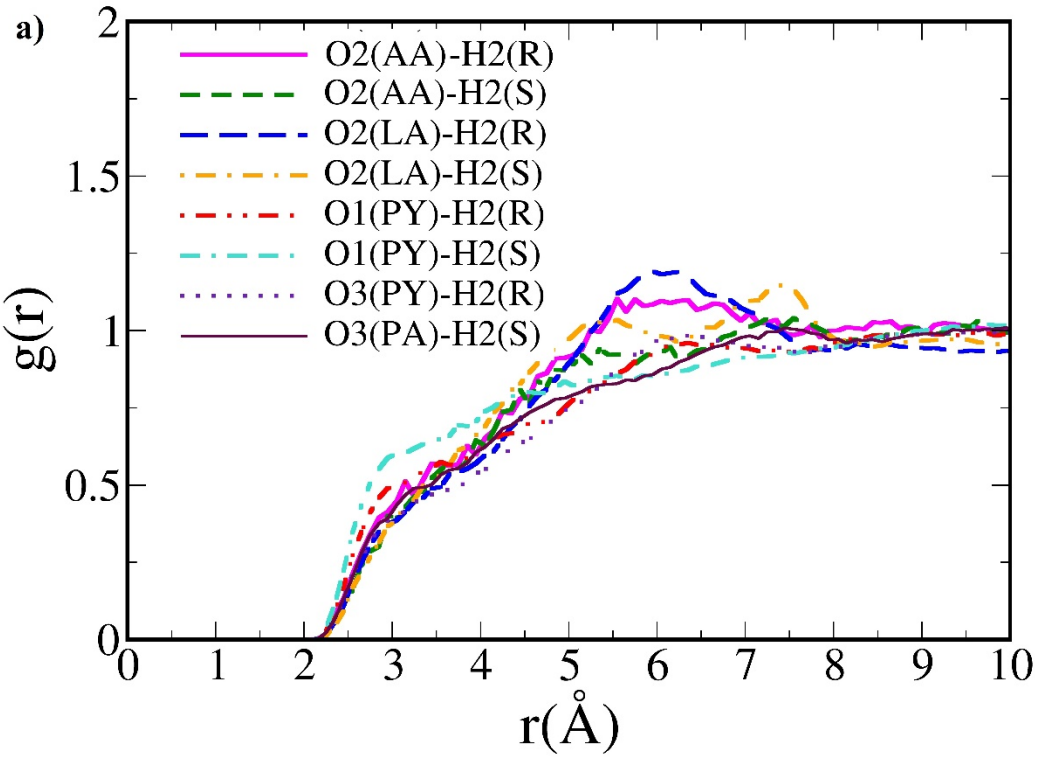
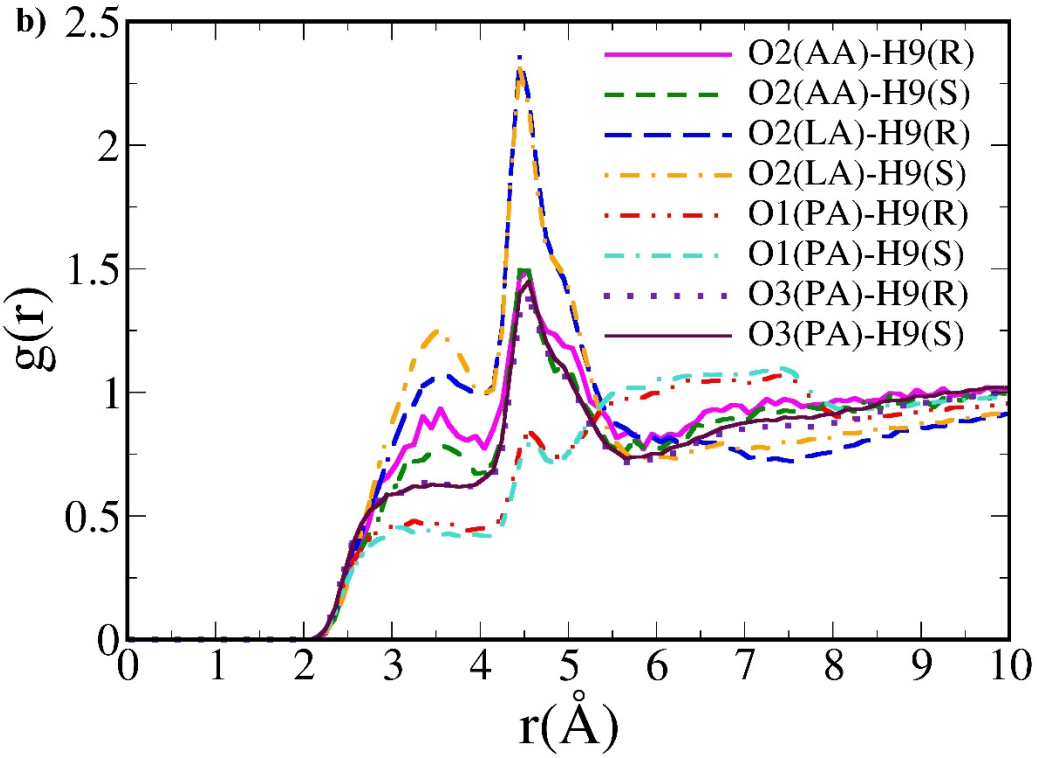


Figure S2. The radial distribution function of the alky hydrogen of DLM (H2) around the carbonyl oxygen of acids, (a); the cyclic hydrogen of DLM (H9) around the carbonyl oxygen of acids, (b); and the alkyl hydrogen of DLM (H15) around the carbonyl oxygen of acids, (c).




b)
g(r)
r(Å)
O2(AA)-H9(R)
O2(AA)-H9(S)
O2(LA)-H9(R)
O2(LA)-H9(S)
O1(PA)-H9(R)
O1(PA)-H9(S)
O3(PA)-H9(R)
O3(PA)-H9(S)

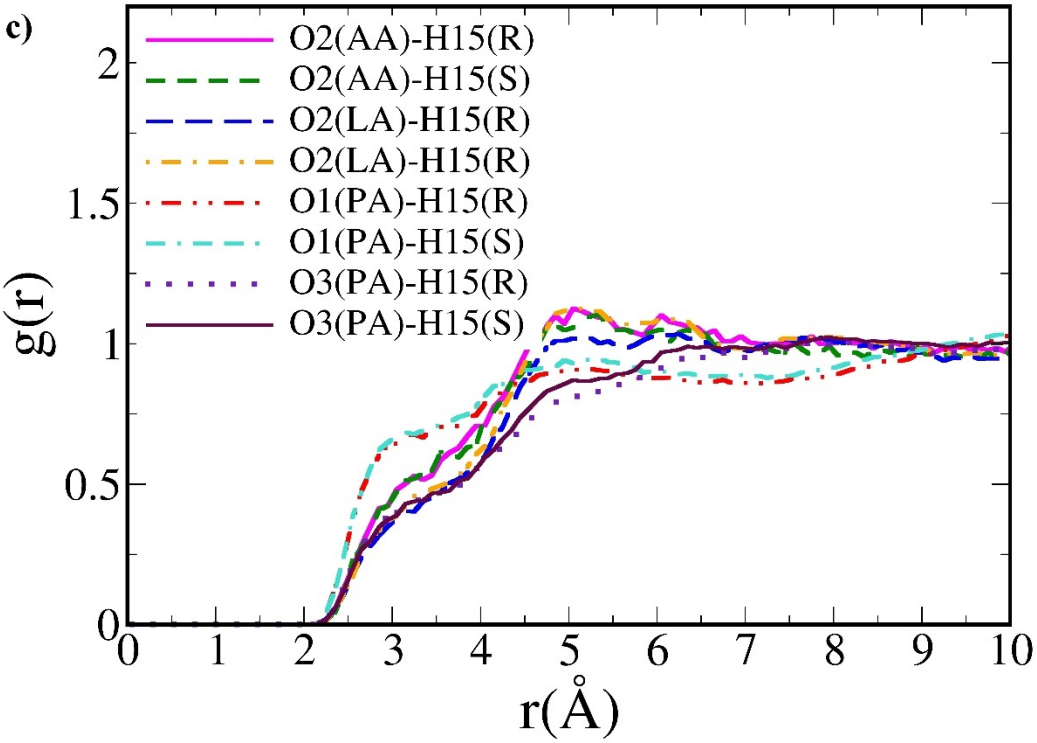
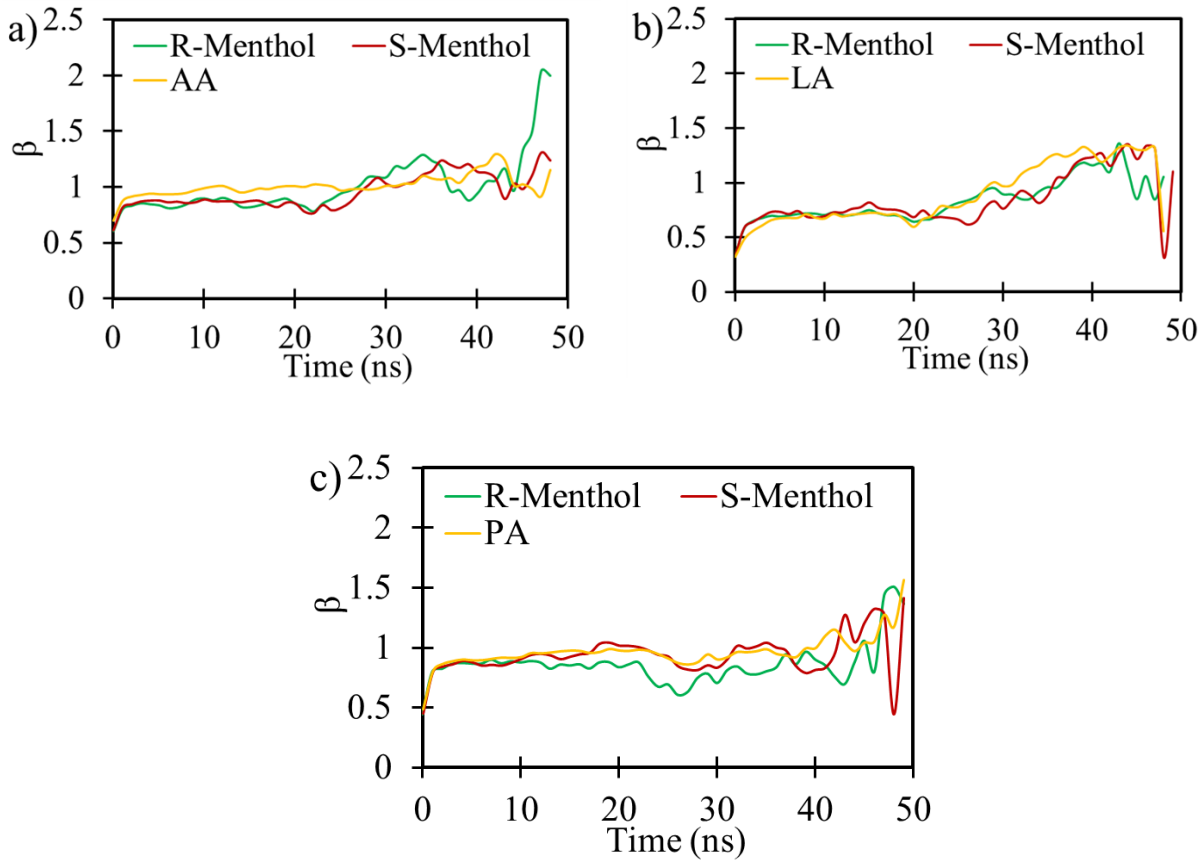

c)
g(r)
r(Å)
O2(AA)-H15(R)
O2(AA)-H15(S)
O2(LA)-H15(R)
O2(LA)-H15(R)
O1(PA)-H15(R)
O1(PA)-H15(S)
O3(PA)-H15(R)
O3(PA)-H15(S)

Figure S3. The assessment of beta parameter for DES1; a, DES2; b, and DES3; c.



Tables:

Table S1. The partial charges and vdW parameter for R ad S-menthol.

Atom type of R ad S-menthol	Partial charges of R ad S-menthol	ε_i (kcal/mol)	σ_i (Å)
C1, C3	-0.1636	0.055	4.35
C2	0.1219	0.055	4.35
C4	-0.0023	0.055	4.35
C5	-0.0973	0.055	4.35
C6	-0.0699	0.055	4.35
C7	0.0943	0.055	4.35
C8	-0.1901	0.055	4.35
C9	-0.1531	0.055	4.35
C10	-0.0921	0.055	4.35
O1	-0.6921	0.1521	3.54
H1, H2, H3, H5, H6, H7	0.0358	0.022	2.64
H4	-0.0003	0.022	2.64
H8	0.0622	0.022	2.64
H9, H10	0.0360	0.022	2.64
H11, H12	0.0286	0.022	2.64
H13	0.0100	0.022	2.64
H14, H15, H16	0.0425	0.022	2.64
H17, H18	0.0889	0.022	2.64
H19	0.0618	0.022	2.64
H20	0.4407	0.0460	0.449

Table S2. The partial charges and vdW parameter for acetic acid.

Atom type of acetic acid	Partial charges of AA	ε_i (kcal/mol)	σ_i (Å)
C1	-0.2913	0.055	4.35
C2	0.8099	0.11	4
O1	-0.6621	0.152	3.540
O2	-0.6025	0.1200	3.40
H1, H2, H3	0.0978	0.022	2.64
H4	0.4526	0.046	0.449

Table S3. The partial charges and vdW parameter for lauric acid.

Atom type of lauric acid	Partial charges of lauric acid	ε_i (kcal/mol)	σ_i (Å)
C1	0.7793	0.11	4.00
C2	-0.0456	0.055	4.35
C3	-0.0109	0.055	4.35
C4	0.0086	0.055	4.35
C5	0.0095	0.055	4.35
C6, C10	0.0103	0.055	4.35
C8	0.0235	0.055	4.35
C9	0.0028	0.055	4.35
C11	0.0332	0.055	4.35
Cl2	-0.0768	0.055	4.35
O1	-0.6954	0.1521	3.54
O2	-0.6108	0.1200	3.40
H1, H2	0.0392	0.022	2.64
H3, H4	0.0111	0.022	2.64
H5, H6	-0.0048	0.022	2.64
H7, H8	0.0006	0.022	2.64
H9, H10	-0.0050	0.022	2.64
H11, H12	-0.0066	0.022	2.64
H13, H14	-0.0103	0.022	2.64
H15, H16	-0.0059	0.022	2.64
H17, H18	-0.0004	0.022	2.64
H19, H20	-0.0023	0.022	2.64
H21, H22 H23	0.0154	0.022	2.64
H24	0.4700	0.046	0.449

Table S4. The partial charges and vdW parameter for pyravic acid.

Atom type of pyravic acid	Partial charges of pyravic acid	ε_i (kcal/mol)	σ_i (Å)
C1	-0.2071	0.055	4.35
C2	0.5187	0.11	4.00
C3	0.6937	0.11	4.00
O1	-0.4801	0.12	3.40
O2	-0.6783	0.1521	3.54
O3	-0.5479	0.12	3.40
H1, H2, H3	0.0735	0.022	2.64
H4	0.4805	0.046	0.449

Table S5. The simulated and experimental density (in g/cm^3**)** of the studied systems at 298.15 K.

Species	Systems		
	DES1	**DES2**	**DES3**
	Density (g/cm^3)		
Simulated	0.942±0.008	0.915±0.002	1.006±0.007
Experimental	0.931	0.894	0.995
Deviation	1.18%	2.35%	1.10%
	Viscosity (mPa.s)		
Simulated	9.83	36.25	31.81
Experimental	8.69	24.42	29.95
Deviation	13.12%	48.44%	6.21%

Table S6. Coordination number (N_{i-j}) of Gly, and choline around the Cl through different sites. The N_{i-j} indicate the coordination number of jth species around ith species.

N_{i-j}	First min position (Å)	DES Type		
		DES1	DES2	DES3
$N_{H18(R)-O=C}$	2.75	0.228	0.292	0.072
				0.115
$N_{H18(S)-O=C}$	2.75	0.245	0.328	0.076
				0.125
$N_{H18(R)-OH(Acid)}$	2.55	0.027	0.031	0.012
$N_{H18(S)-OH(Acid)}$	2.55	0.022	0.041	0.012
$N_{HO(Acid)-OH18(R)}$	2.75	0.229	0.282	0.180
$N_{HO(Acid)-OH18(S)}$	2.75	0.204	0.288	0.180
$N_{H15(R)-O=C}$	3.55	0.081	0.053	0.082
				0.050
$N_{H15(S)-O=C}$	3.55	0.082	0.056	0.081
				0.050
$N_{H9(R)-O=C}$	4.05	0.227	0.219	0.097
				0.130
$N_{H9(S)-O=C}$	4.05	0.198	0.241	0.091
				0.129
$N_{H2(R)=O=C}$	3.35	0.056	0.040	0.046

				0.037
$N_{H2(S)=O=C}$	3.35	0.050	0.040	0.055
				0.039

Table S7. The diffusion coefficient of species (in $Å^2$/ns**)** of the studied systems.

Species	Systems		
	DES1	**DES2**	**DES3**
	Diffusion coefficient ($Å^2$/ns)		
S-menthol	1.148±0.008	0.222±0.002	0.6526±0.007
R-menthol	1.174±0.01	0.227±0.002	0.8126±0.002
Acetic acid	3.376±0.01	---	---
Lauric acid	---	0.294±0.001	---
Pyravic acid	---	---	1.464±0.004