Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplemental Data

The relationship between enhanced enzyme activity and structural dynamics in ionic liquids: a combined computational and experimental study

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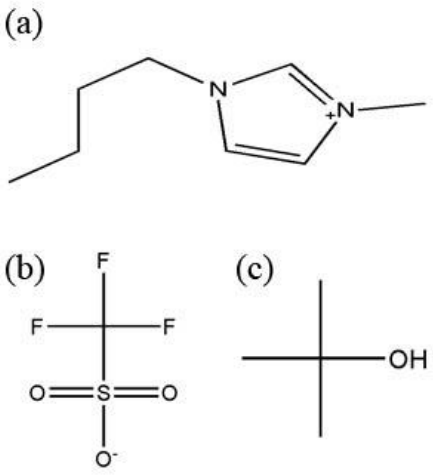

Figure S1. Chemical structure of solvents used in this study. (a) 1-Butyl-3-methylimidazolium ($[Bmim]^+$), (b) Trifluoromethanesulfonate ($[TfO]^-$) and (c) *tert*-butanol.

Table S1. Simulation set-up.

Solvent	Components	Number of Ions / Molecules[a]	Volume of Simulation Box[b] ($Å^3$)
[Bmim][TfO]	$[Bmim]^+$	452	596,523
	$[TfO]^-$	451	
tert-butanol	Na^+	1	636,935
	tert-butanol	1,444	
[Bmim][Cl]	$[Bmim]^+$	494	694,954
	Cl^-	493	
0.3M NaCl solution	Water	10,543	454,682
	Na^+	82	
	Cl^-	81	

[a] One cation ($[Bmim]^+$, or Na^+) was additionally added into system to neutralize charge of system.
[b] Distance between any atom of enzyme and the edge of periodic box is at least 10 Å.

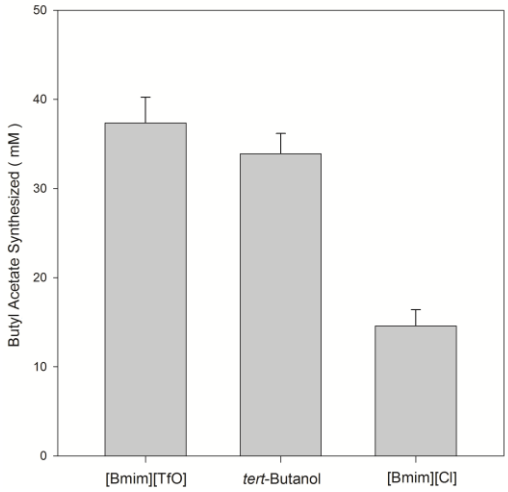

Figure S2. The production yield of butyl acetate after 12 h reaction in [Bmim][TfO], *tert*-butanol and [Bmim][Cl].

Table S2. The average of initial reaction rate of lipase-catalyzed trans-esterification of butyl alcohol with vinyl acetate in [Bmim][TfO], *tert*-butanol, [Bmim][Cl].

Solvent	Initial Reaction Rate (mM / hr)
[Bmim][TfO]	0.863
tert-butanol	0.619
[Bmim][Cl]	0.153

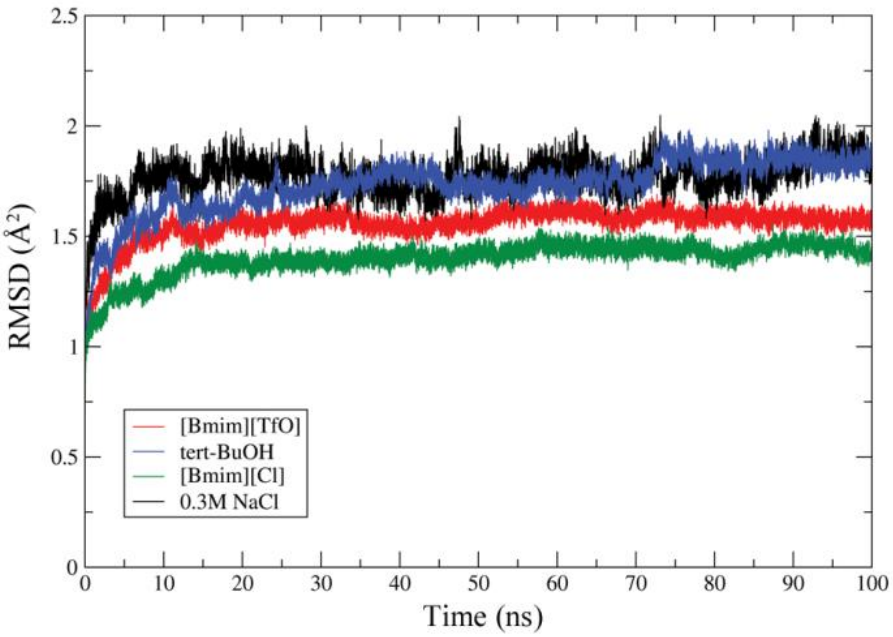

Figure S3. Root mean square deviation (RMSD) of CALB that was calculated for backbone atoms as a function of time during 100 ns in [Bmim][TfO] (Red), *tert*-butanol (Blue), [Bmim][Cl] (Green), and 0.3M NaCl solution (Black).

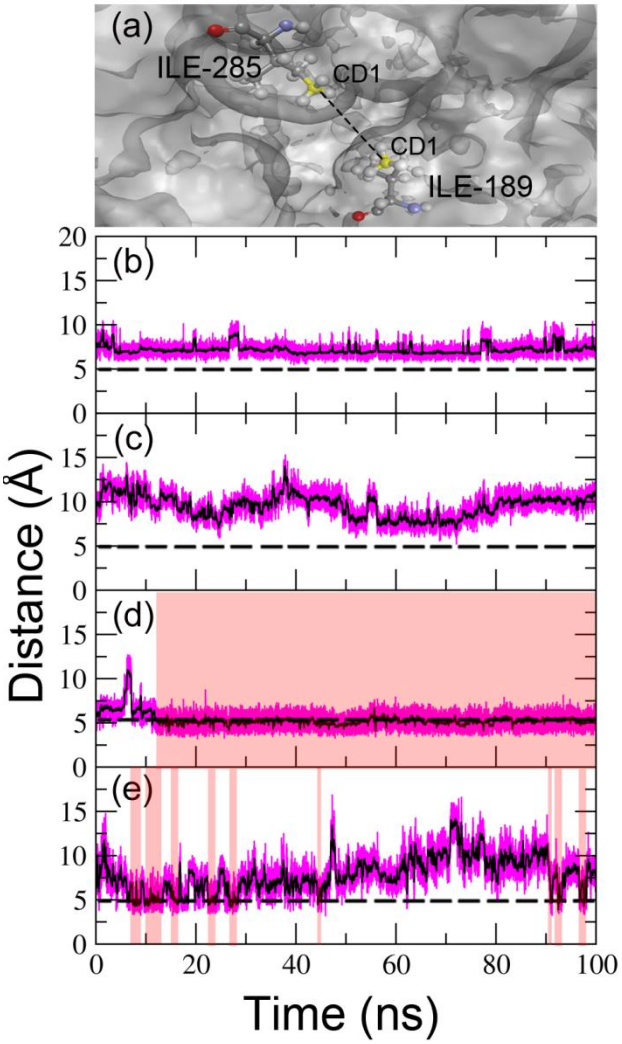

Figure S4. (a) Snapshot of CD1 atoms of ILE-189 and ILE-285, and (b-e) temporal profiles of the distance between CD1 atoms in ILE-189 and ILE-285 in (b) [Bmim][TfO], (c) *tert*-butanol, (d) [Bmim][Cl], and (e) 0.3M NaCl. Average profile is shown as black line. A black dotted line indicates the threshold distance for closed conformation and red shading indicates time periods when the distance is less than 5 Å.

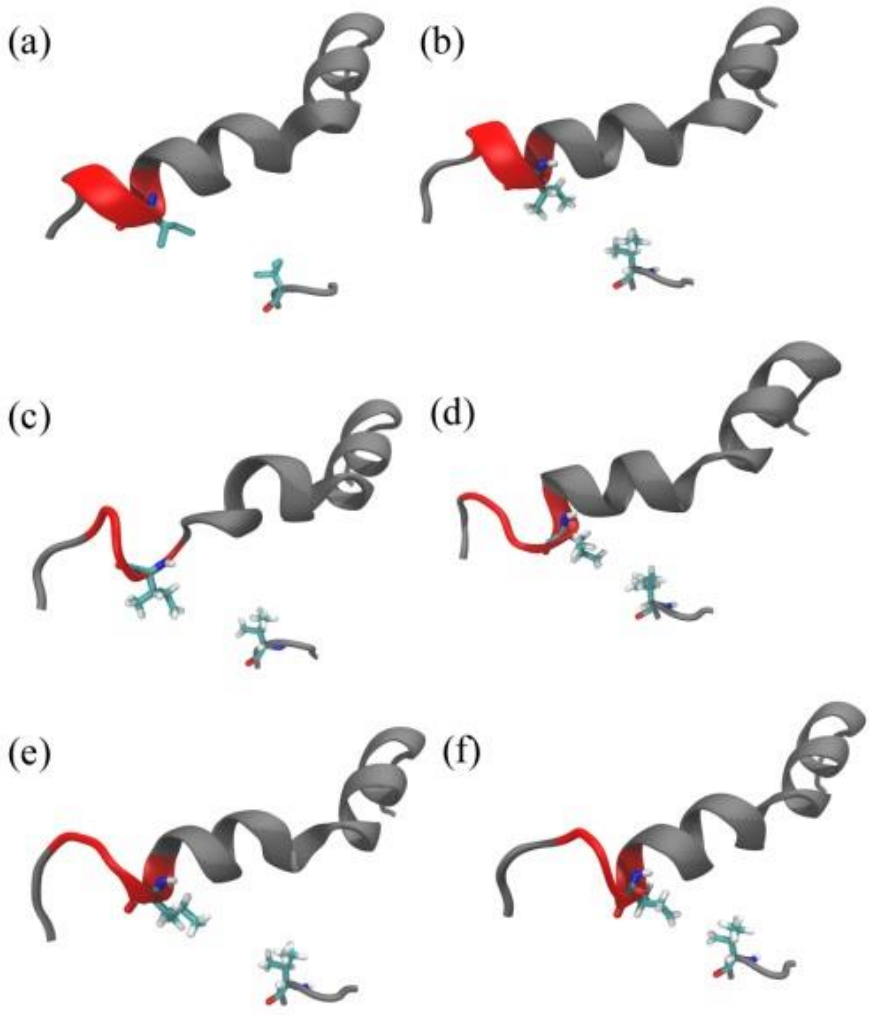

Figure S5. Conformational changes of the alpha-10 helix region in various solvents (a) initial X-ray crystal structure, (b) [Bmim][TfO], (c) *tert*-butanol, (d) [Bmim][Cl], (e) 0.3M NaCl (Open), (f) 0.3M NaCl (Closed). Region with significant conformational changes is shown in red. ILE-189 and ILE-285 are shown as stick molecular model.

Table S3. The number of anions that interact with CALB and the average non-bonded energy between CALB and one anion.

	Number of anions that interact with CALB[a]	Non-bonded energy between an anion and CALB[b] (kcal/mol)
[Bmim][TfO]	55	-53.372
[Bmim][Cl]	37	-102.646

[a] within 2.5 Å from surface of CALB
[b]Non-bonded energy = electrostatic energy + Van der Waals contribution