Supporting Information

for

Role of Imidazolium Cation on Structure and Activity of *Candida antarctica* Lipase B Enzyme in Ionic Liquids

Ho Shin Kim, Doyoung Eom, Yoon-Mo Koo, and Yaroslava G. Yingling

[1]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695-7907 (USA)

[2]Department of Biological Engineering, Inha University, Incheon 402-751 (Republic of Korea)

Table S1. Simulation setup

Solvent	Components	Molecular Volume ($Å^3$)	Volume Ratio V_a/V_c	Volume of Simulation Box ($Å^3$)	Density from MD (g /ml)	Density from experiment (g / ml)
[Emim][TfO]	$[Emim]^+$	234.25	0.71	192,151.21 (±121.28)	1.39	1.39[1]
	$[TfO]^-$	165.70				
[Bmim][TfO]	$[Bmim]^+$	296.77	0.56	205,552.22 (±109.61)	1.32	1.30[2]
	$[TfO]^-$	165.70				
[Hmim][TfO]	$[Hmim]^+$	360.29	0.46	251,349.19 (±204.87)	1.25	1.20[1]
	$[TfO]^-$	165.70				
[Omim][TfO]	$[Omim]^+$	423.70	0.39	277,985.43 (±83.18)	1.21	1.19[3]
	$[TfO]^-$	165.70				

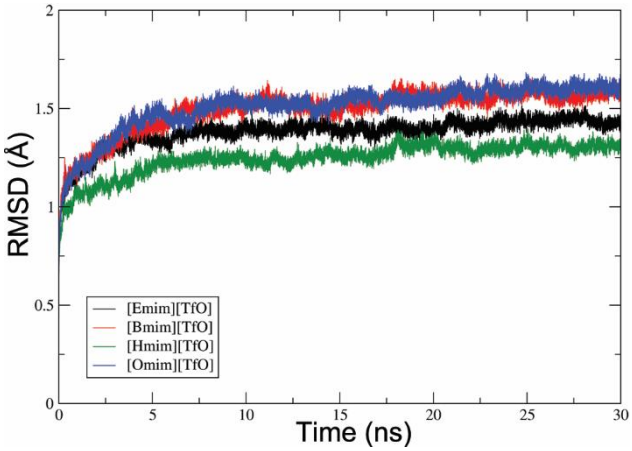

Figure S1. Root mean square deviation (RMSD) of CALB solvated in [Emim][TfO] (black), [Bmim][TfO] (Red), [Hmim][TfO] (Dark green) and [Omim][TfO] (Blue)

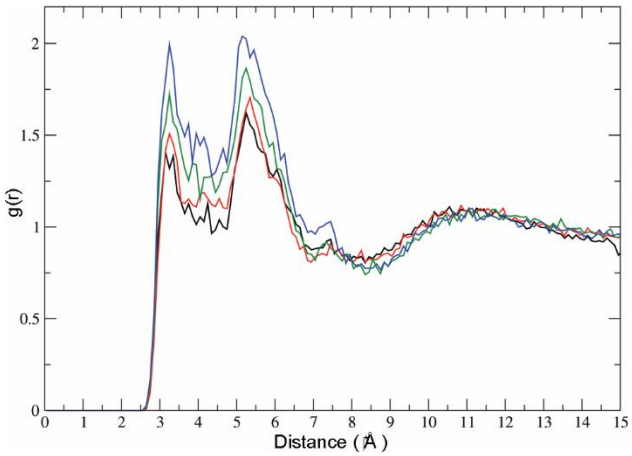

Figure S2. Radial distribution function of carbon atom in imidazolium cation. $[Emim]^+$ (black), $[Bmim]^+$ (red), $[Hmim]^+$ (green), and $[Omim]^+$ (blue). Second solvation shell (7 Å) is used for estimation of coordination number.

Table S2. Reaction rate of butyl acetate synthesis reaction using CALB in ILs

Solvents	Reaction Rate (mol / L·hr)
[Emim][TfO]	0.20
[Bmim][TfO]	0.85
[Hmim][TfO]	0.77
[Omim][TfO]	0.74

Table S3. Secondary structure of α-10 helix (residue 285 to 287) in ILs

CALB in	Residue	3-10 Helix	Alpha Helix	Turn
[Emim][TfO]	285 ILE	1.469	83.668	13.756
	286 VAL	6.258	62.206	25.974
	287 ALA	6.312	27.957	42.023
[Bmim][TfO]	285 ILE	0.043	99.887	0.370
	286 VAL	0.037	99.196	0.764
	287 ALA	0.086	80.785	11.383
[Hmim][TfO]	285 ILE	0.697	99.141	0.162
	286 VAL	0.025	98.581	1.394
	287 ALA	0.019	90.414	5.123
[Omim][TfO]	285 ILE	0.021	95.418	4.540
	286 VAL	0.127	94.087	5.744
	287 ALA	0.127	70.626	17.115

Each percentage value was calculated in consecutive frame of 30 ns simulations

References

(1) A. Berthod, M. Ruiz-Angel and S. Carda-Broch, J. Chromatogr. A, 1184, 6 (2008).
(2) S. H. Lee and S. B. Lee, Chem. Commun., 3469 (2005).
(3) S. H. Ha, N. L. Mai and Y.M. Koo, Process. Biochem., 45, 1899 (2010).