

Recovery of enzyme structure and activity following rehydration from ionic liquid

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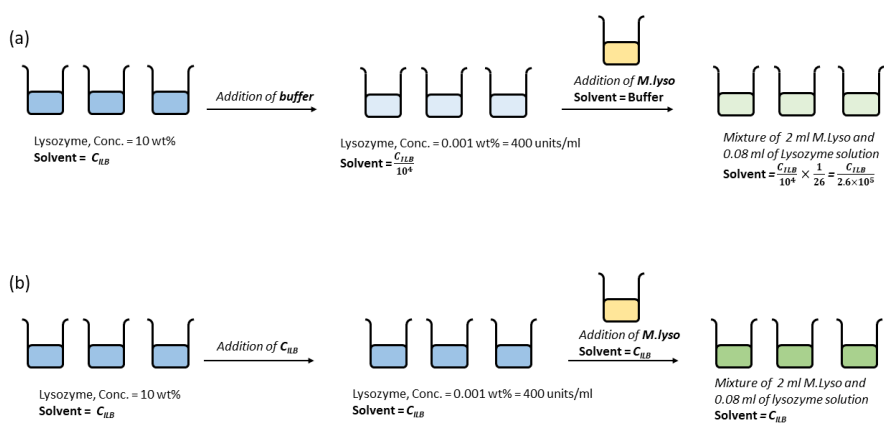


Figure S1: Schematic of activity assays. (a) "Traditional" assay where samples are diluted with phosphate buffer to achieve required final enzyme concentration of 400 U/mL. (b) "Modified" assay where samples are prepared and mixed at a constant composition, C_{ILB} refers to IL-buffer mixture from 5% to 17% IL.

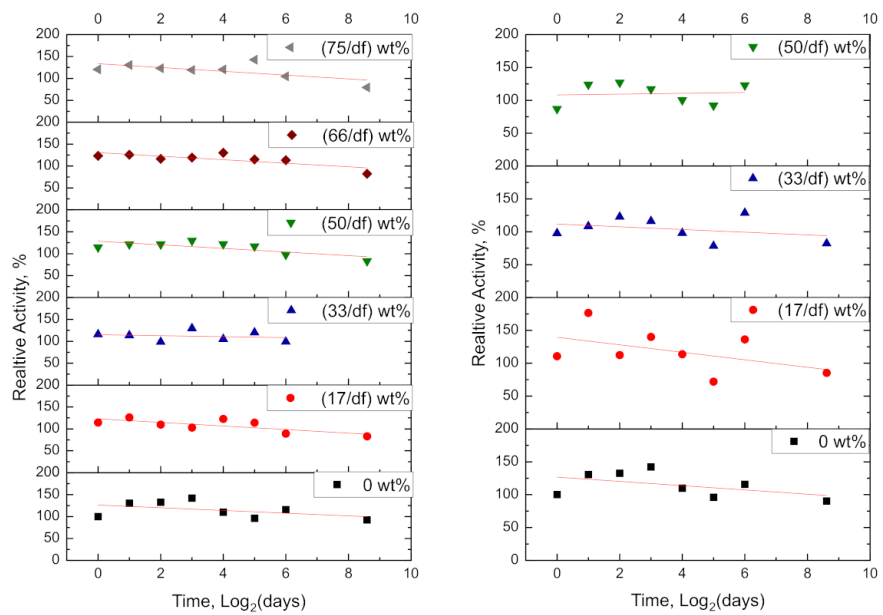


Figure S2: Lysozyme activity after rehydration, following different storage times in IL-water mixtures. The dilution factor $df = 2.6 \times 10^5$. Left: [EMIM][EtSO₄]. Right: [EMIM][Et₂PO₄]

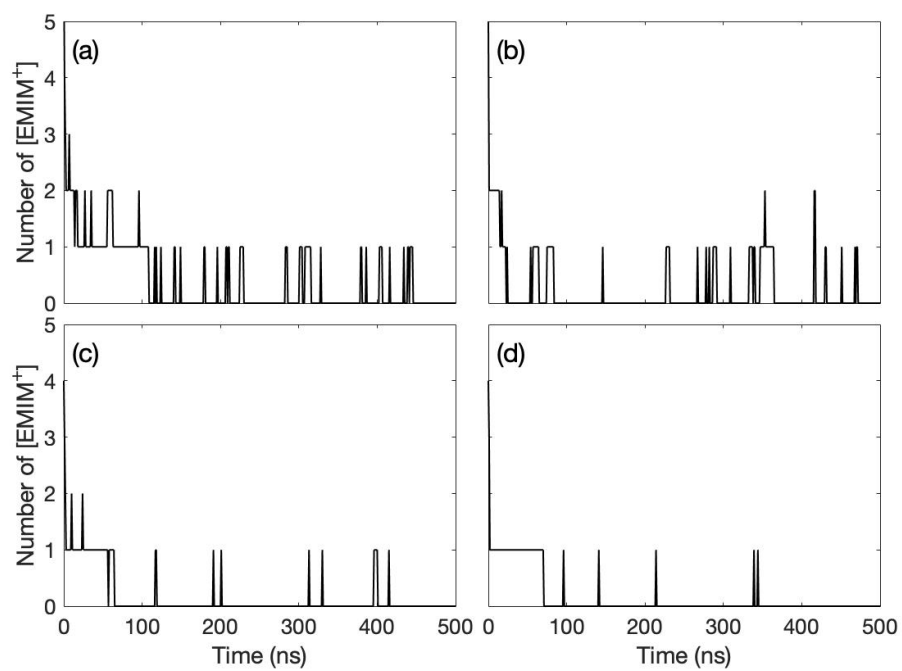


Figure S3: The time series showing the number of [EMIM⁺] molecules near the non-native ligand binding site for (a) rehydrated [EMIM][EtSO₄] system replica 2, (b) rehydrated [EMIM][EtSO₄] system replica 3, (c) rehydrated [EMIM][Et₂PO₄] system replica 2, and rehydrated [EMIM][Et₂PO₄] system replica 3.

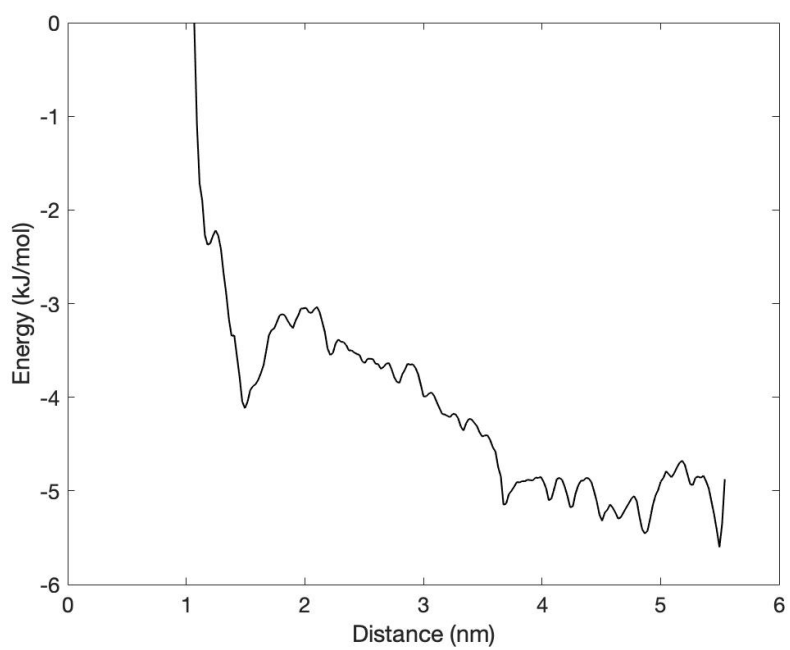


Figure S4: Umbrella sampling simulations showing the PMF plot for the distance of an [EMIM⁺] molecule away from the lysozyme along the pulling direction in a hydrated system.

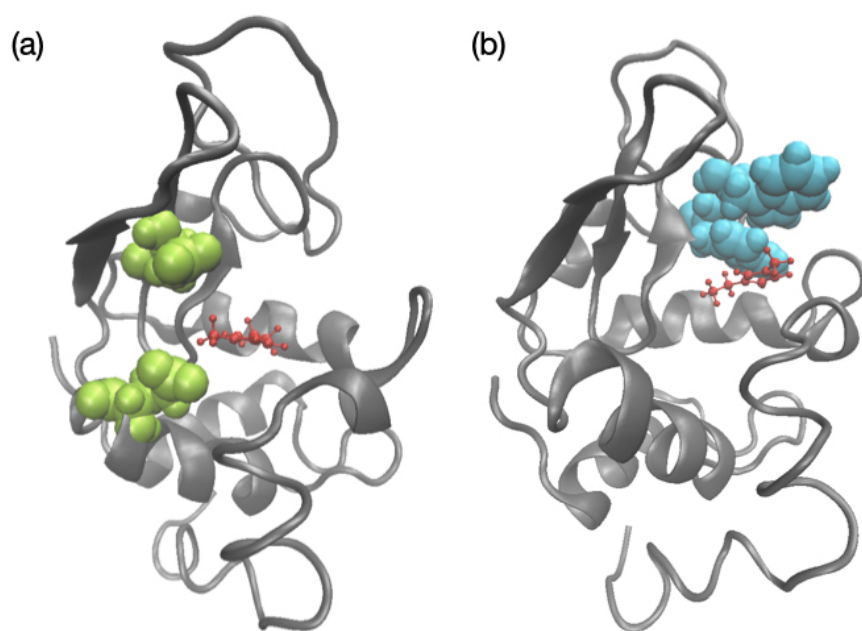


Figure S5: Illustration showing the close contact between an [EMIM⁺] molecule (red) and (a) the active site residues (green) (b) TRP62/63 residues (cyan).