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Lid Dynamics of Porcine Pancreatic Lipase in Non-aqueous Solvents

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Keywords: pancreatic lipase; lid opening; molecular simulation; water; octanol.

Abbreviations: PPL-Cl, procine pancreatic lipase in closed conformation; PPL-O, lipase in closed conformation; PPL^{+colip}, lipase-colipase complex; PPL^{-colip}, only lipase chain of lipase-colipase complex; PPL_{mut}-Cl, lipase with point mutations D250V and E254 in closed conformation; RMSD – root mean square deviation; RMSF – root mean square fluctuation; R_g – radius of gyration; SASA – solvent accessible surface area; PCA – principal component analysis; RMSIP - root mean square inner product.

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