

Supplementary Materials

Brown Spider Venom Phospholipase-D Activity upon Different Lipid Substrates

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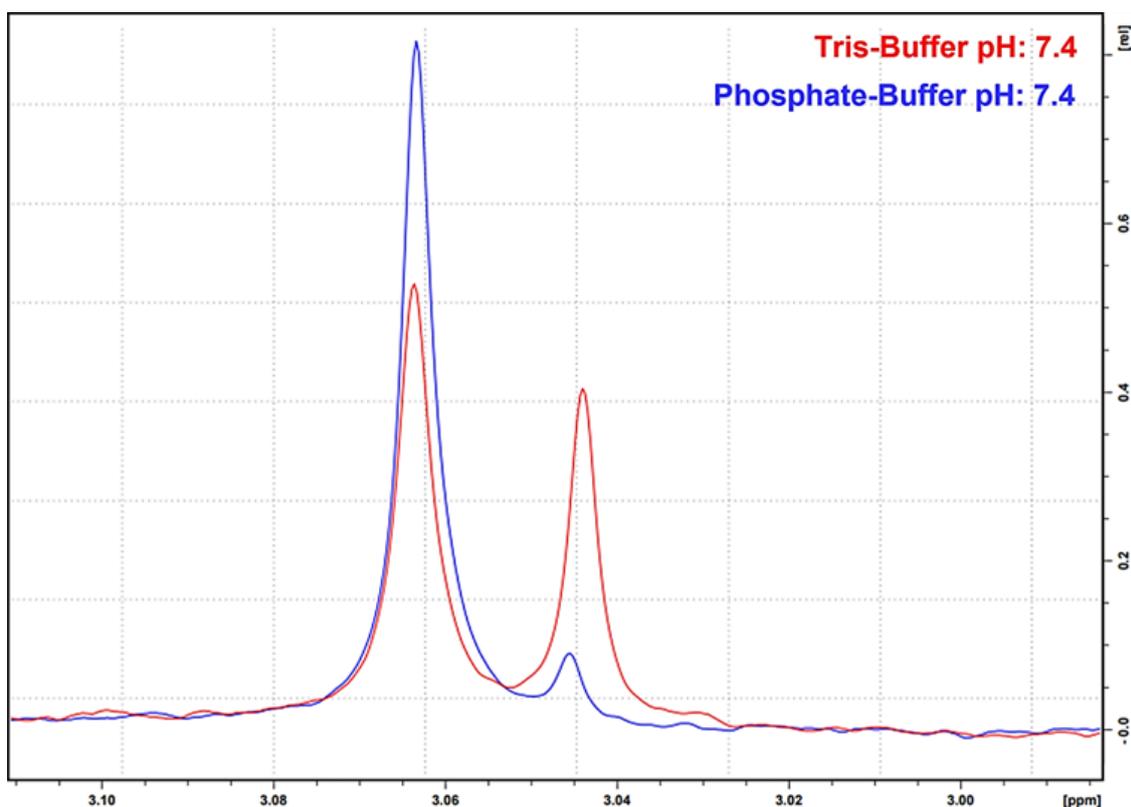


Figure S1. One dimensional ¹H-NMR spectra of -CH₂- resonance of buffers used in NMR spectroscopy experiments whose results are shown in Figures S2 and S3.

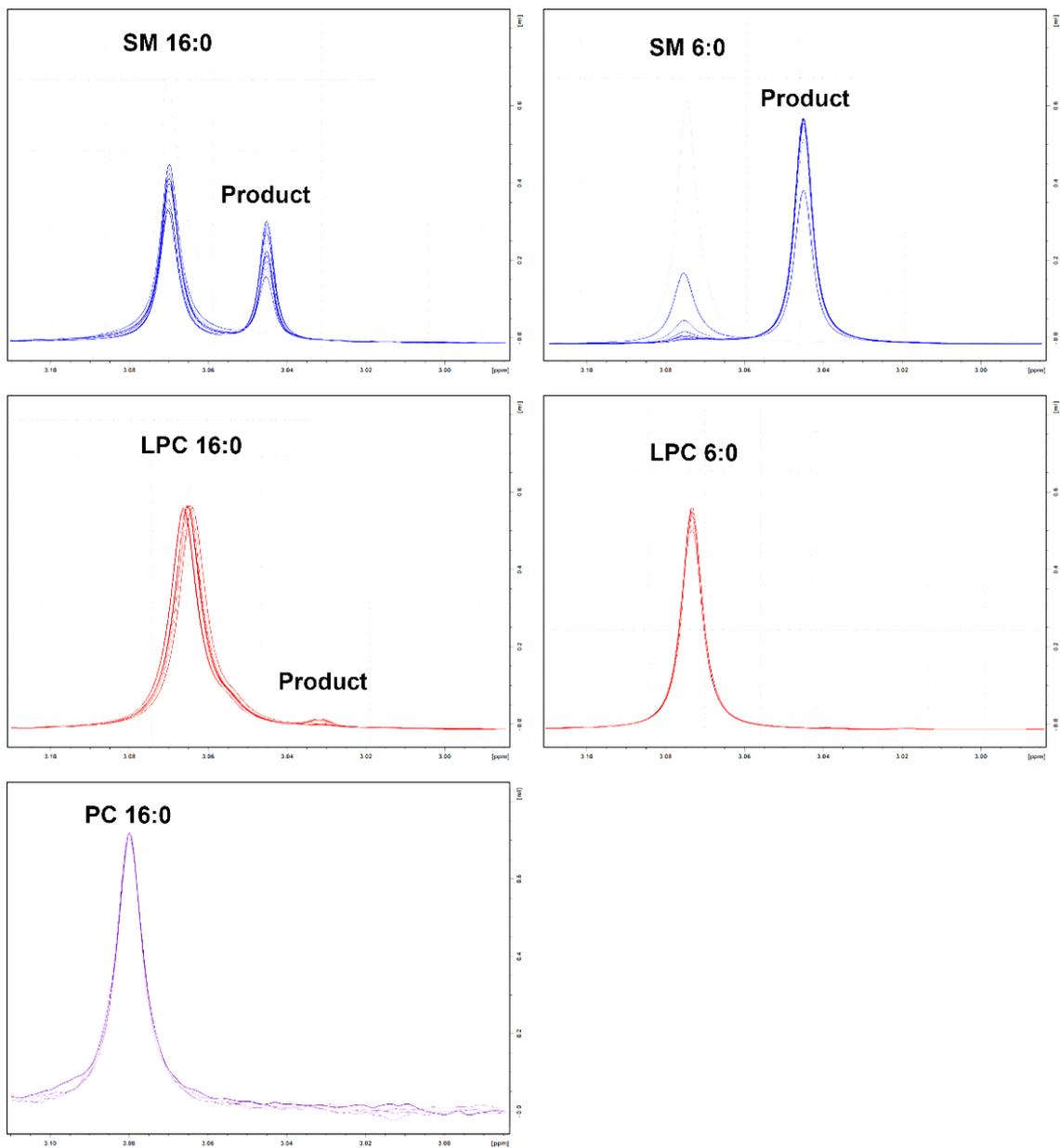


Figure S2. Analysis of the cleavage activity of Brown spider recombinant phospholipase-D (LiRecDT1) on different phospholipid substrates, studied by using NMR spectroscopy. A) One dimensional ^1H -NMR spectra of $-\text{CH}_2-$ resonance of SM 16:0, SM 6:0, LPC 16:0, LPC 6:0 and PC 16:0 monitored along a 2-hour period after recombinant phospholipase-D treatment.

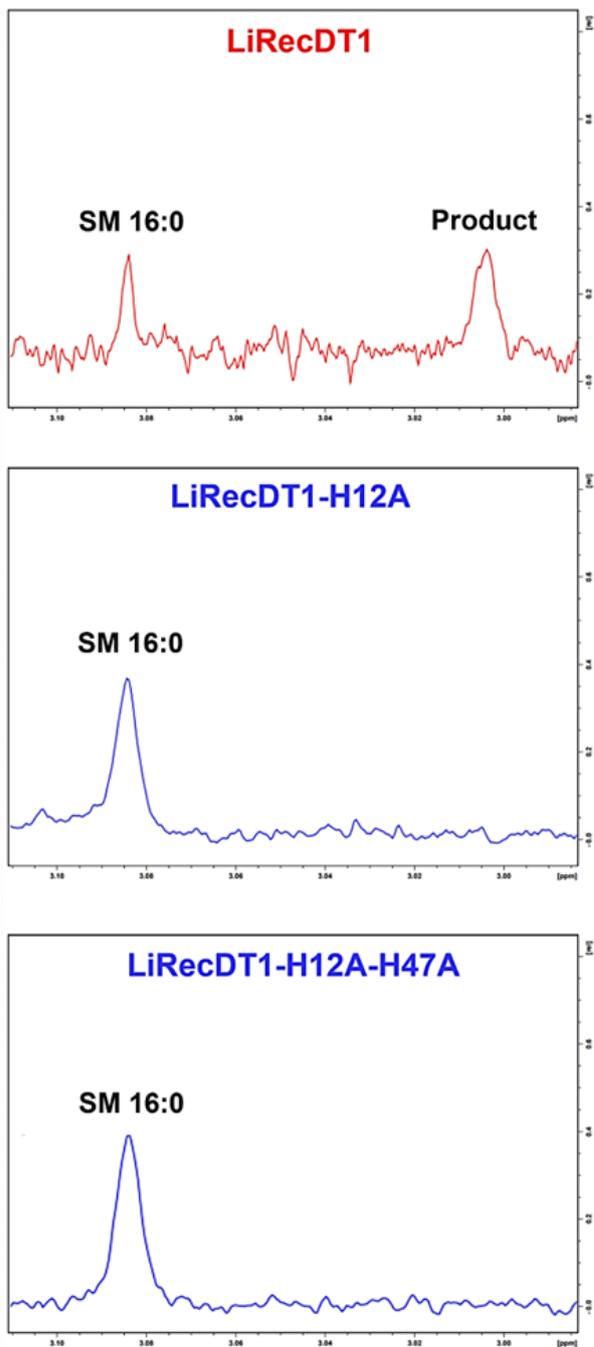


Figure S3. Analysis of the cleavage activity of Brown spider recombinant wild-type or mutated phospholipases-D on SM 16:0, studied by using NMR spectroscopy. A) One dimensional ^1H -NMR spectra of $-\text{CH}_2-$ resonance of SM 16:0 incubated with LiRecDT1 (wild-type), LiRecDT1-H12A and LiRecDT1-H12A-H47A (mutations in amino acid residues of catalytic site) monitored along a 2-hour period after recombinant phospholipase-D treatment.

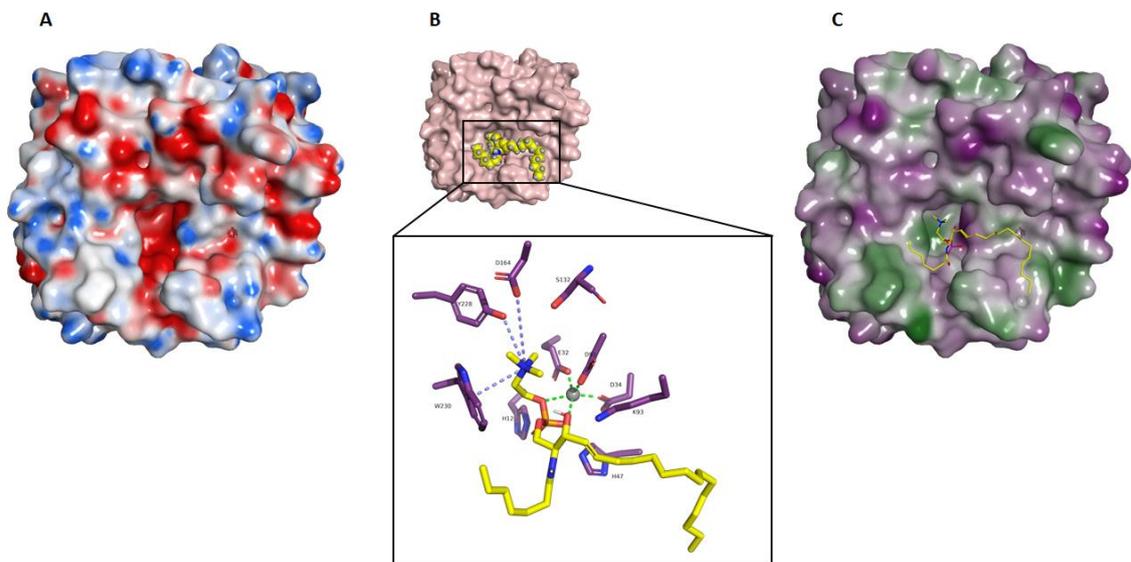


Figure S4. Structural analysis of brown spider recombinant phospholipase-D with sphingomyelin SM 06:0. **(A)** Molecular surface with electrostatics determined by Poisson-Boltzmann method showing deep electronegative substrate binding cleft of *L. intermedia* PLD. Electrostatic color map range from -40 (red) to +40 (blue). **(B)** Molecular surface representation of *L. intermedia* PLD with **SM 06:0** (d18:1/06:0) docked substrate shown as solid space-filled spheres (yellow) and close-up view of the docked pose. **(C)** Molecular surface of *L. intermedia* PLD docked with **SM 06:0** (d18:1/06:0) substrate colored by hydrophobicity (green) and hydrophilicity (purple).