Modeling protein-micelle systems in implicit water

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SUPPORTING INFORMATION

Table S1. Average RMSD values from three independent 5-ns simulations

Micelle System	Protein Name	RMSD (Å) run 1	RMSD (Å) run 2	RMSD (Å) run 3
DPC	Magainin 2	1.2 ± 0.3	1.1 ± 0.3	1.1 ± 0.3
	ARP1	1.2 ± 0.2	1.3 ± 0.3	1.2 ± 0.2
	GP41	1.6 ± 0.4	1.7 ± 0.4	1.0 ± 0.4
SDS	Magainin 2	1.0 ± 0.2	1.0 ± 0.2	1.0 ± 0.2
	ARP1	1.2 ± 0.2	1.2 ± 0.3	1.2 ± 0.3

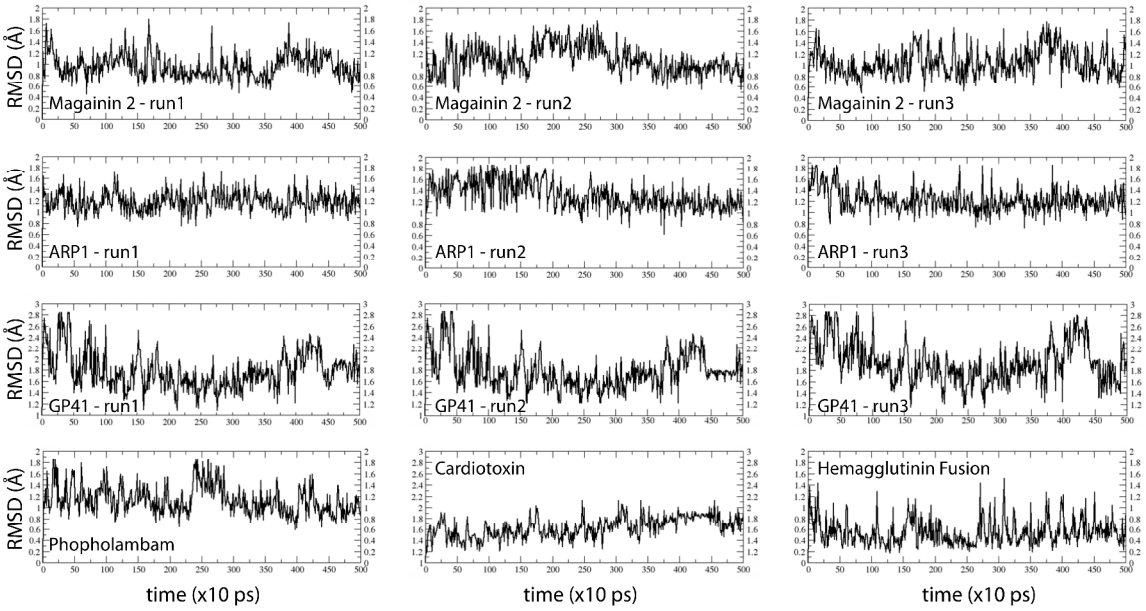

Figure S1. Time evolution of the RMSD value of the protein against its NMR structure for 5 ns in DPC micelles.

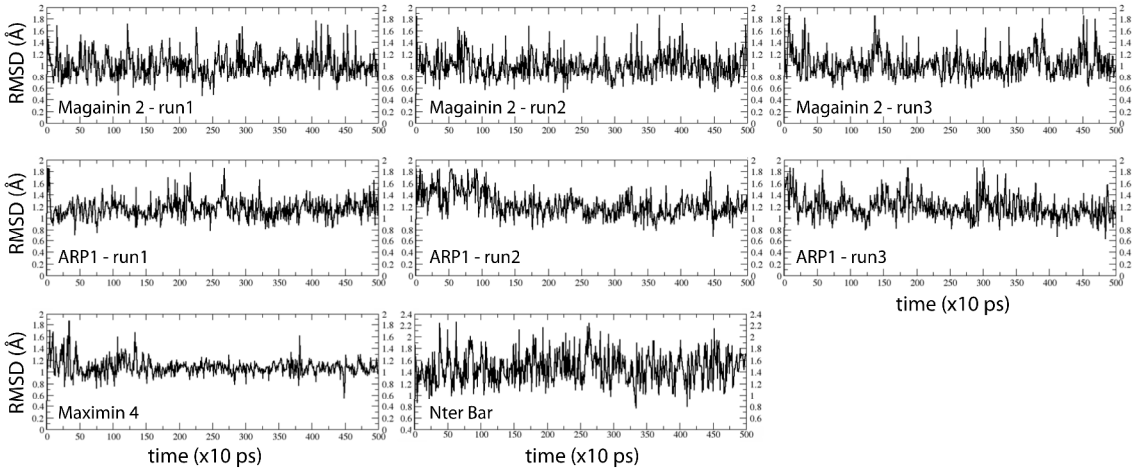

Figure S2. Time evolution of the RMSD value of the protein against its NMR structure for 5 ns in SDS micelles.

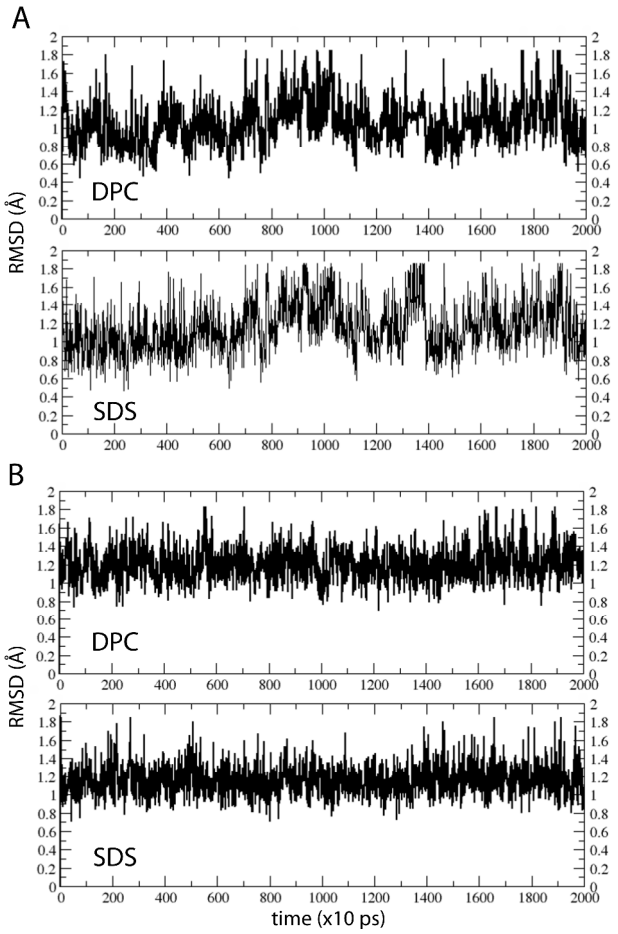

Figure S3. Time evolution of the RMSD value of the protein A) Magainin 2 and B) ARP1 against their respective NMR structure for 20 ns in DPC and SDS micelles.