

Supporting Information

Investigating the Molecular Mechanism by Which Natural Polyamines Alter the Conformational Stability and Dynamics of Lysozyme

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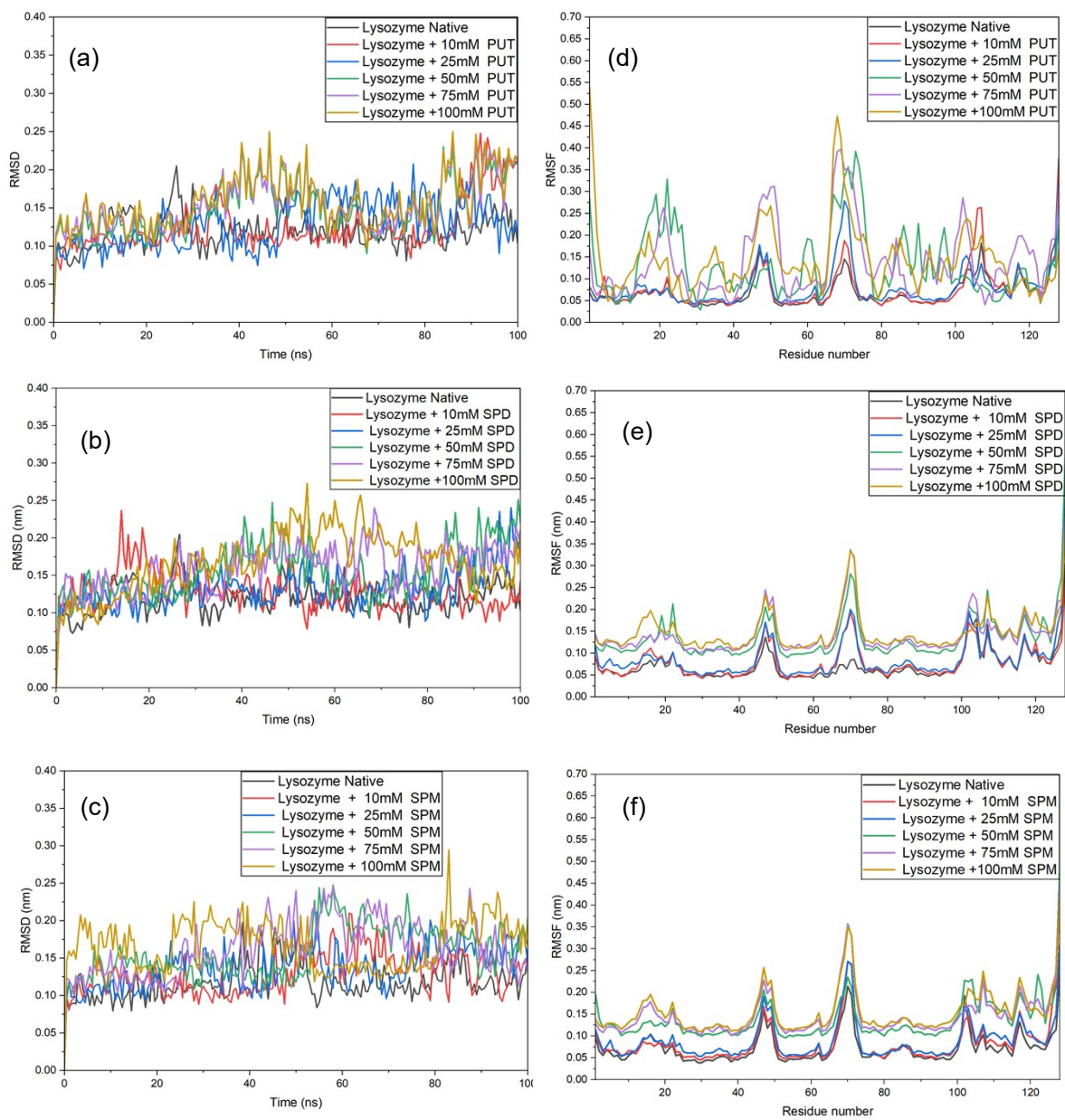


Fig. S1: Panels (A), (B), and (C) represent the RMSD of HEWL in the presence of different concentrations of PUT, SPD, and SPM, respectively, at pH 4.4. Panels (D), (E), and (F) represent the RMSF of HEWL in the presence of different concentrations of PUT, SPD, and SPM, respectively, at a pH of 4.4.

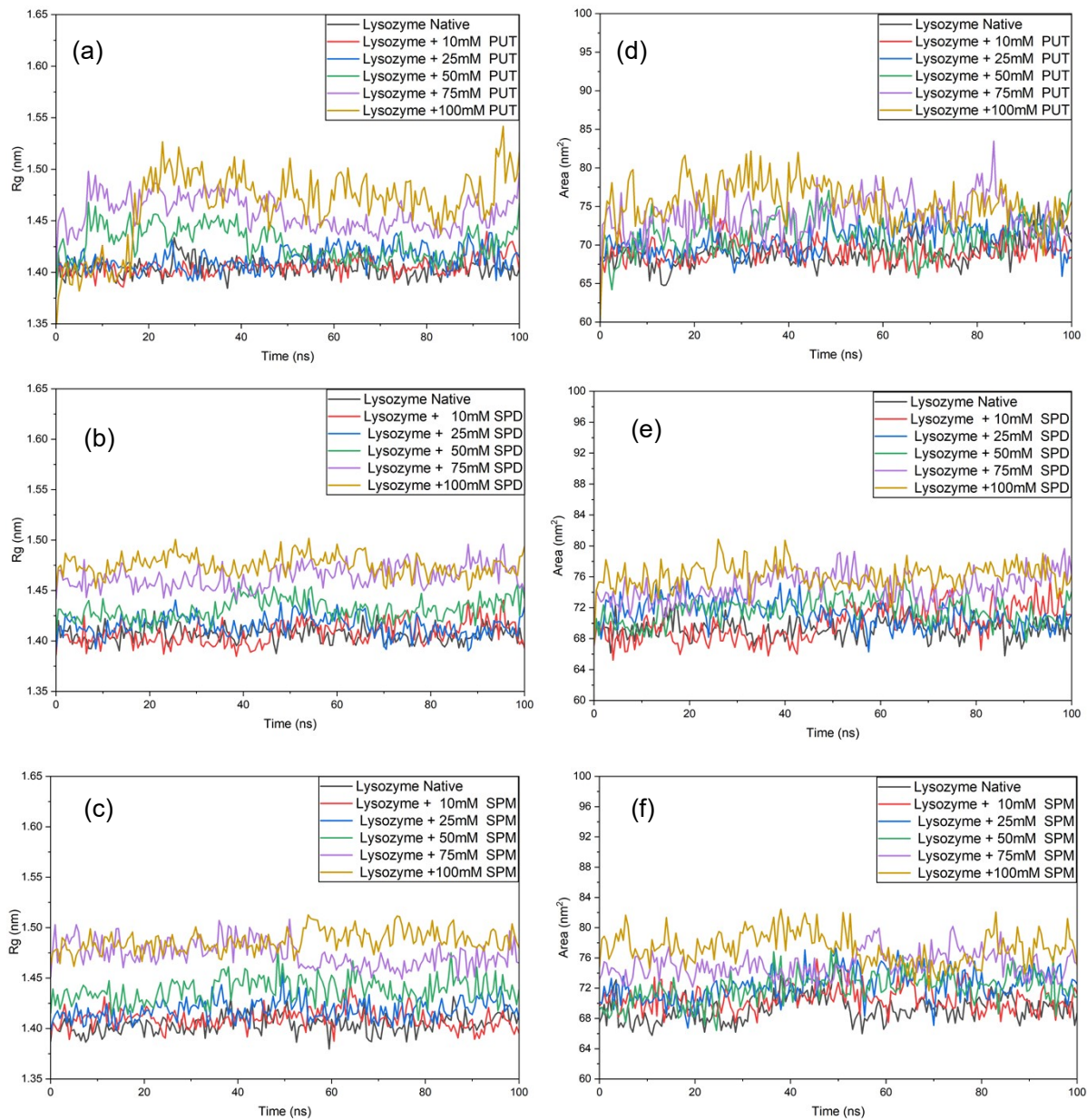


Fig. S2: Panels (A), (B), and (C) represent the R_g values of HEWL in the presence of different concentrations of PUT, SPD, and SPM, respectively, at pH 4.4. Panels (D), (E), and (F) represent the SASA of HEWL in the presence of different concentrations of PUT, SPD, and SPM, respectively, at a pH of 4.4.

Table S1: PAs effect on the average RMSD, R_g , RMSF, SASA, and H-bonds of native HEWL, at pH 4.4

System	Average RMSD (nm)	Average RMSF (nm)	Average R_g (nm)	Average SASA (nm ²)	Average H-bonds (Total H-bonds b/w HEWL and PA)
PUT					
HEWL+0.0 M PAs	0.119±0.023	0.071±0.04	1.404±0.008	69.28±1.73	--
HEWL+10 mM PUT	0.125±0.034	0.076±0.05	1.407±0.006	69.17±1.46	0.02±0.14 (4)
HEWL+25 mM PUT	0.129±0.032	0.080±0.05	1.413±0.011	70.21±1.90	0.09±0.35 (19)
HEWL+50 mM PUT	0.149±0.044	0.131±0.06	1.428±0.016	71.08±2.51	0.70±1.01 (142)
HEWL+75 mM PUT	0.154±0.036	0.139±0.09	1.458±0.016	73.78±2.63	1.59±1.50 (319)
HEWL+100mM PUT	0.158±0.061	0.144±0.08	1.466±0.035	75.46±2.79	3.13±2.14 (630)
SPD					
HEWL +0.0 M PAs	0.119±0.023	0.072±0.07	1.407±0.008	69.27±1.23	--
HEWL+10 mM SPD	0.127±0.025	0.079±0.08	1.408±0.013	69.94±2.19	0.035±0.30 (6)
HEWL+25 mM SPD	0.132±0.027	0.086±0.05	1.415±0.022	71.16±1.70	0.110±0.56 (22)
HEWL+50 mM SPD	0.154±0.035	0.135±0.09	1.431±0.041	71.57±1.63	1.05±1.08 (215)
HEWL+75 mM SPD	0.159±0.031	0.142±0.07	1.464±0.056	74.62±1.90	2.52±1.60 (515)
HEWL+100mM SPD	0.164±0.040	0.149±0.04	1.475±0.010	76.17±1.52	4.18±2.68 (856)
SPM					
HEWL +0.0 M PAs	0.118±0.024	0.072±0.03	1.404±0.008	69.33±1.77	--
HEWL+10 mM SPM	0.129±0.028	0.083±0.05	1.409±0.025	70.56±1.58	0.069±0.45 (8)
HEWL+25 mM SPM	0.136±0.021	0.088±0.04	1.418±0.011	72.36±1.98	0.173±0.83 (35)
HEWL+50 mM SPM	0.157±0.036	0.137±0.05	1.438±0.016	72.00±1.97	1.41±1.36 (288)
HEWL+75 mM SPM	0.162±0.045	0.146±0.08	1.473±0.022	75.11±1.70	2.74±1.27 (560)
HEWL+100mM SPM	0.168±0.036	0.154±0.05	1.486±0.035	77.32±2.06	4.67±3.59 (956)