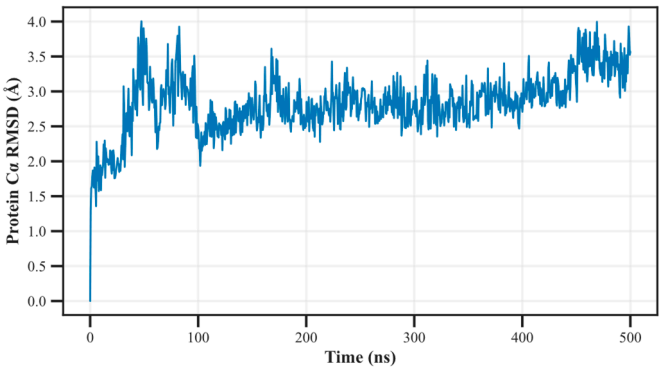
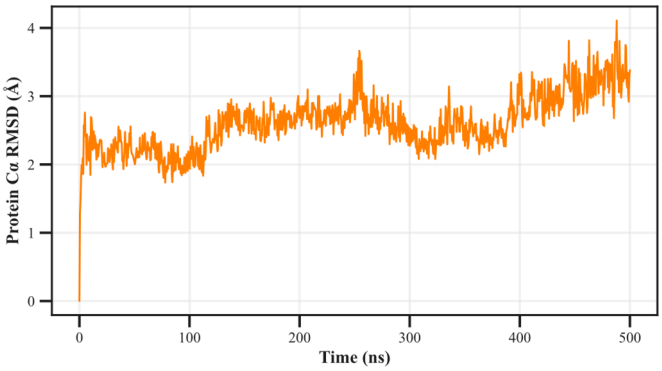
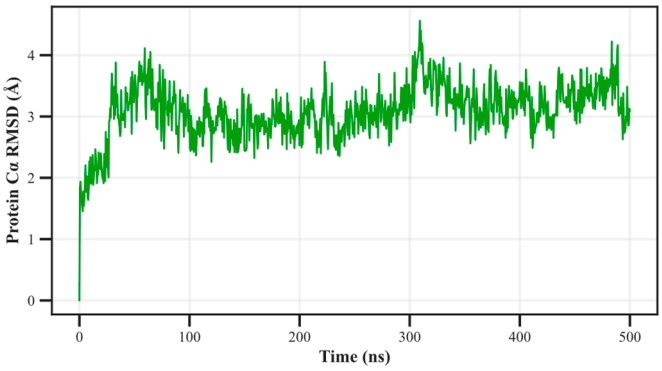
molecules

Supporting Information

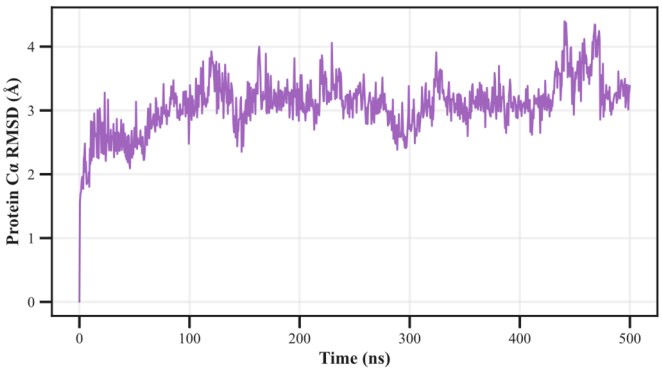
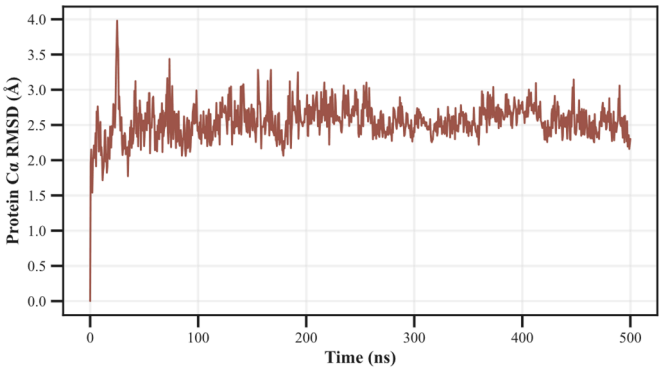
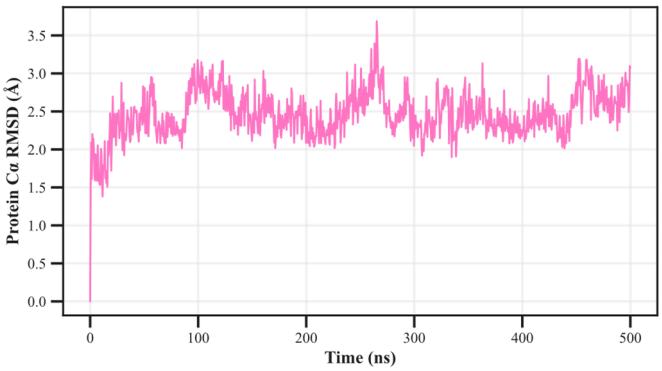
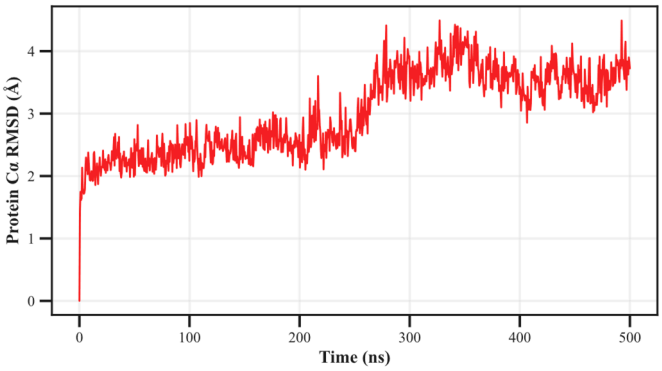
Lipolytic Stimulation and Antioxidant Activity of Saponin-Rich Extracts: Experimental and In Silico Study

Zbigniew Sroka[1,*], Karina Kapusta[2,3], Senal D. Liyanage[3], Ta'Miyia Tobias[3], Victoria Petosyan[3,4], Wojciech Kolodziejczyk[2], Karolina Imiełowska[5], Michał Gleńsk[1], Beata Żbikowska[1], Andrzej Gamian[6], and Kamil Wojciechowski[7]

Figure S1. Protein Root Mean Square Deviation (RMSD) values throughout a 500 ns molecular dynamics simulation for saponin-lipase-colipase complexes.

Ligand	RMSD
Cholate	
Escin Ia	
Hederacoside	

 https://doi.org/10.3390/xxxxx

Ginsenoside Rb1	
Ginsenoside Re	
Ginsenoside Rd	
Ginsenoside Rg1	

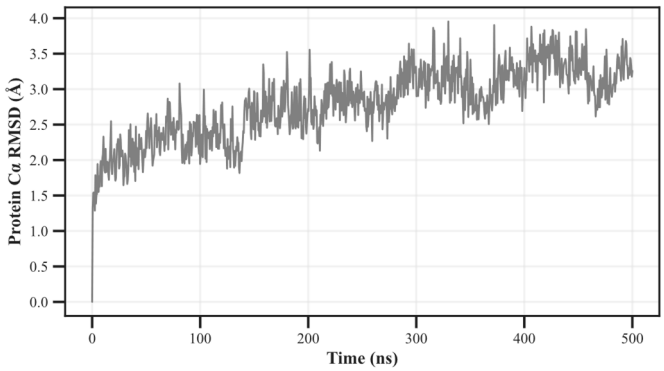
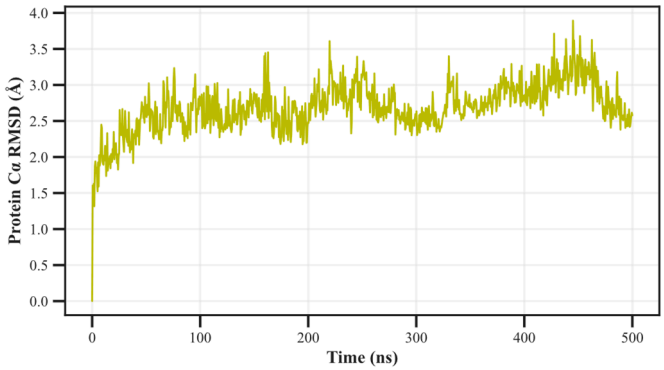
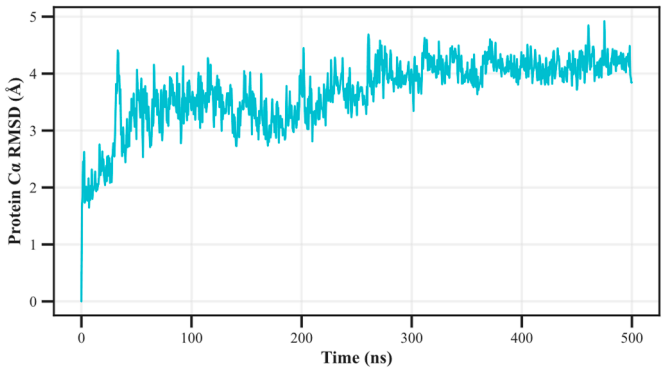
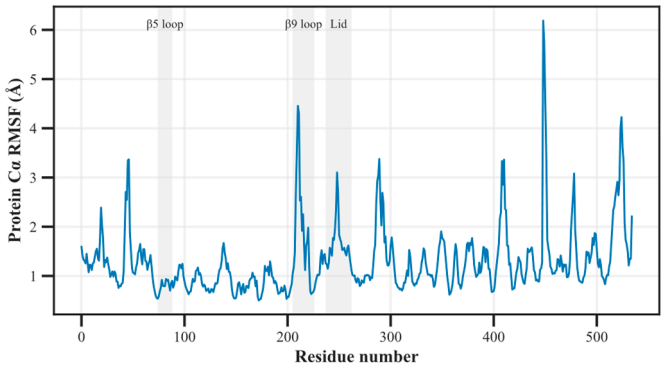
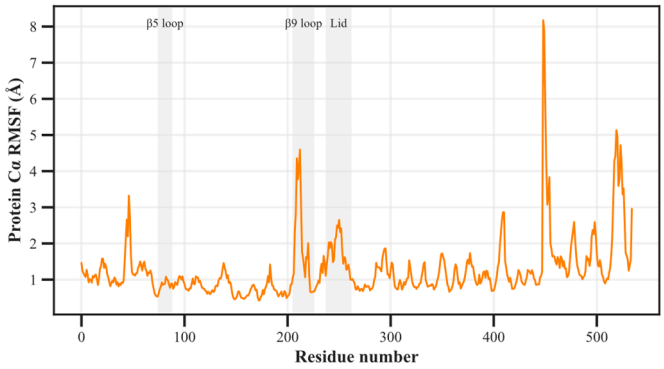
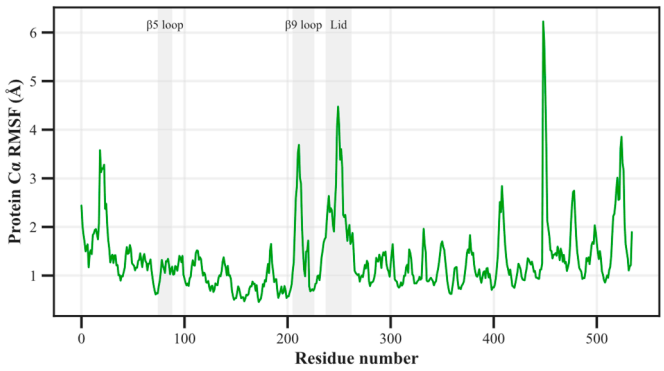
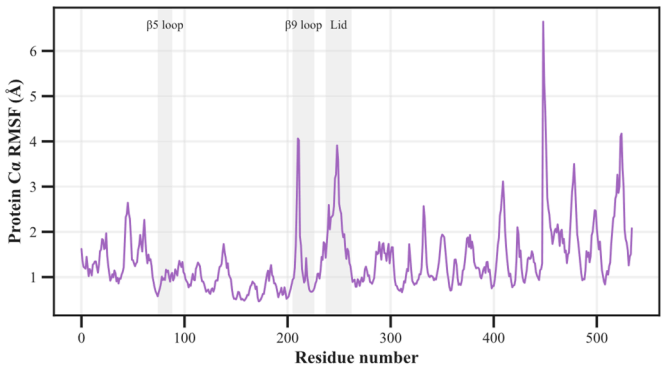
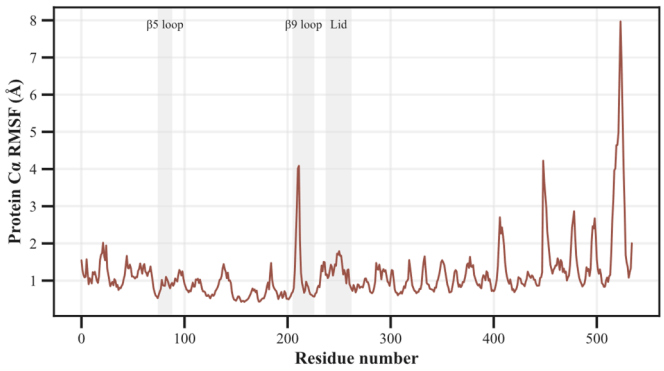
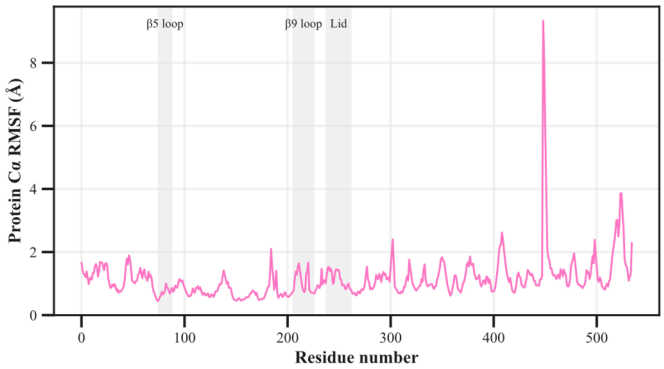
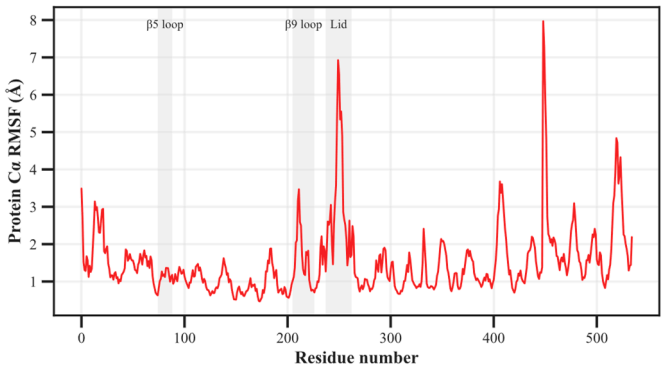
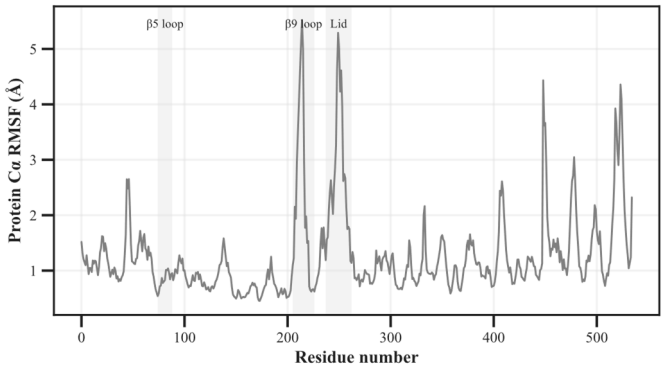
Osladin	
Herniariasaponin 2	
Herniariasaponin 4	

Figure S2. Protein Root Mean Square Fluctuation (RMSF) values throughout a 500 ns molecular dynamics simulation for saponin-lipase-colipase complexes.

Ligand	RMSF
Cholate	
Escin Ia	
Hederacoside	
Ginsenoside Rb1	

Ginsenoside Re	
Ginsenoside Rd	
Ginsenoside Rg1	
Osladin	

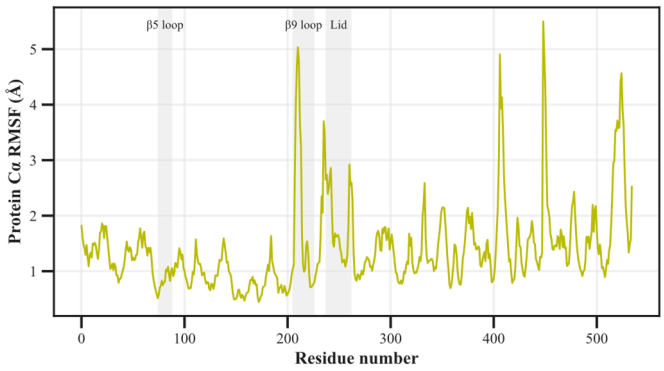
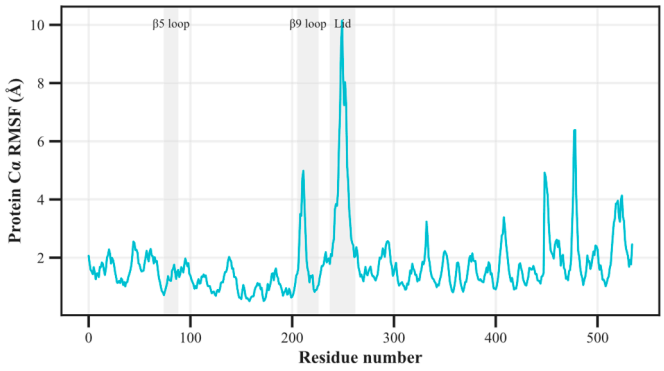
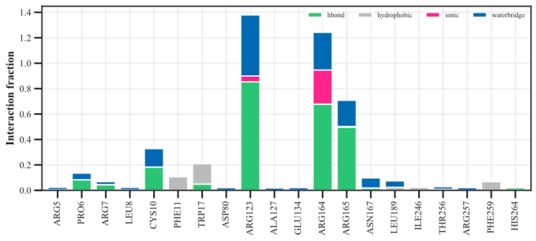
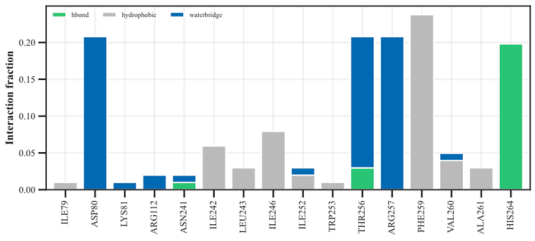
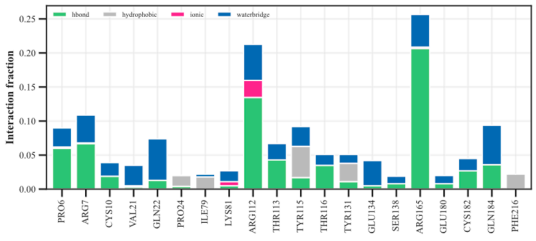
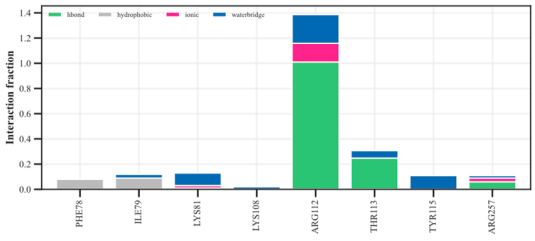
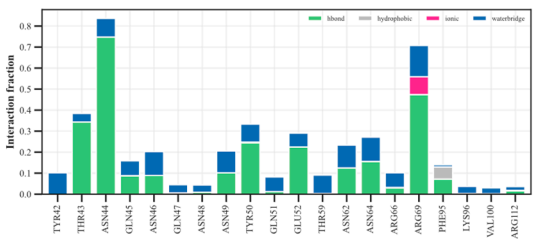
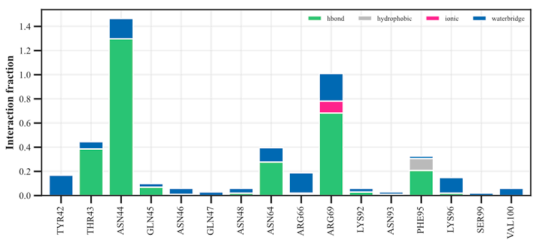
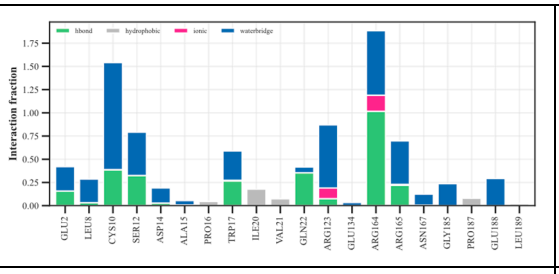
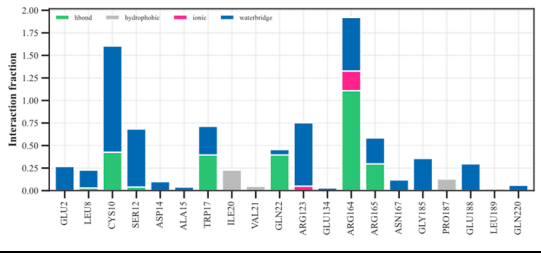
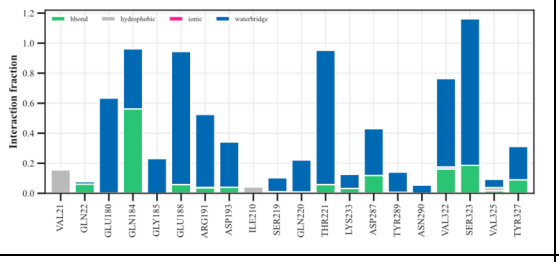
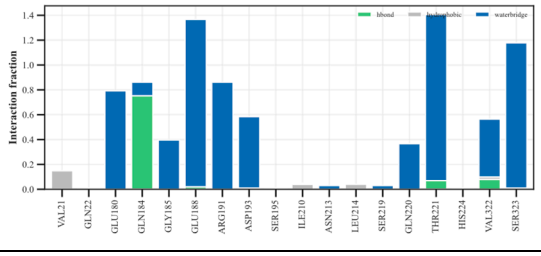
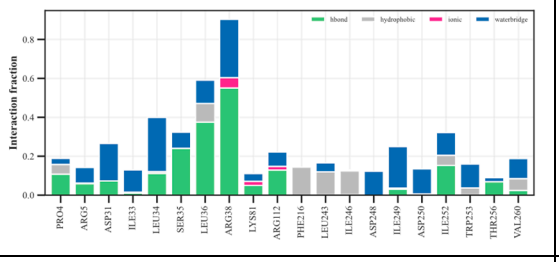
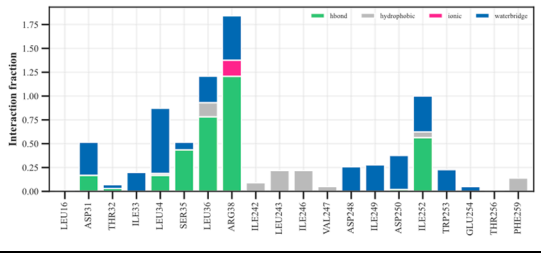
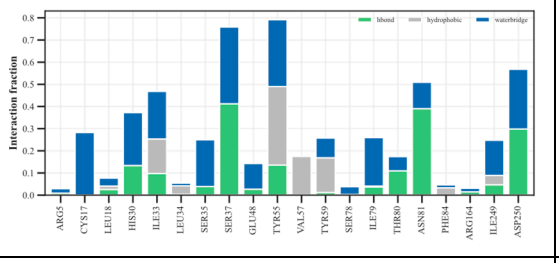
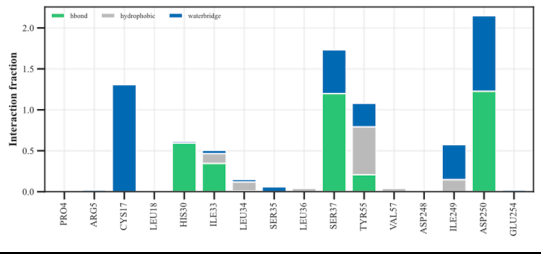
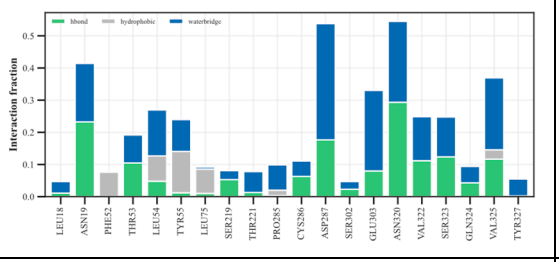
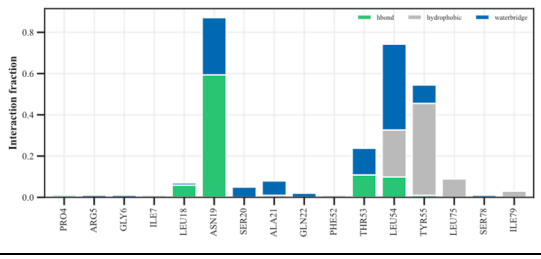
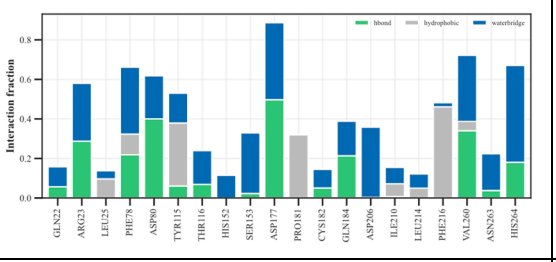
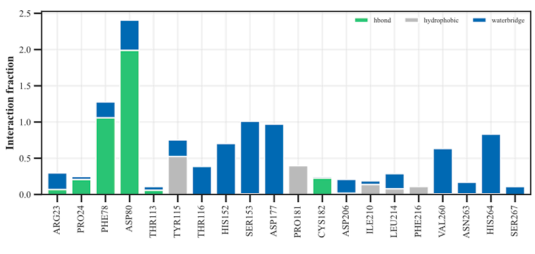
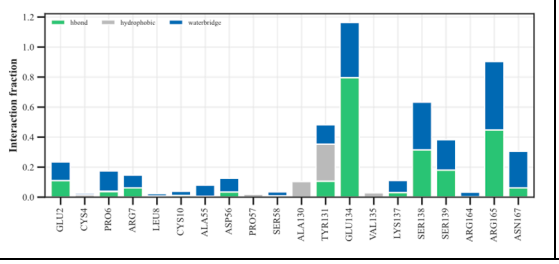
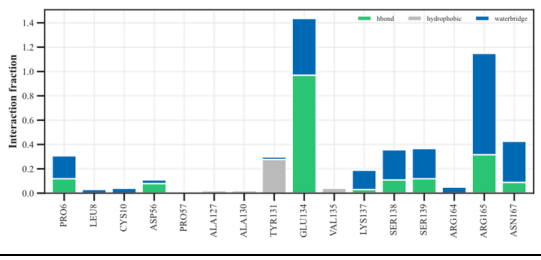
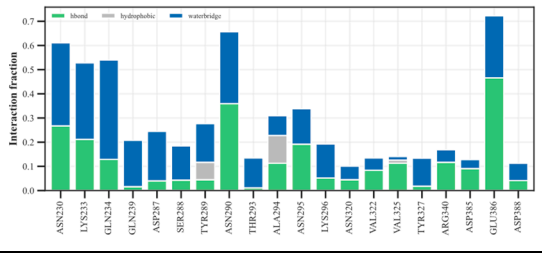
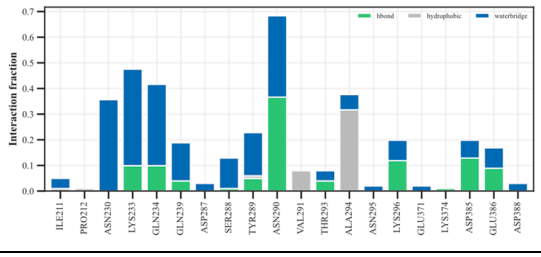
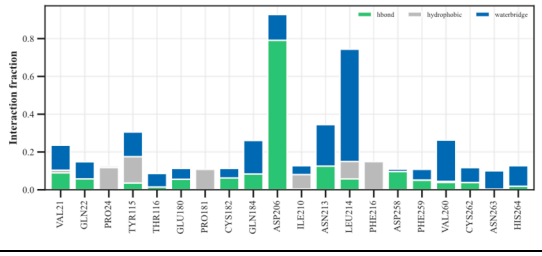
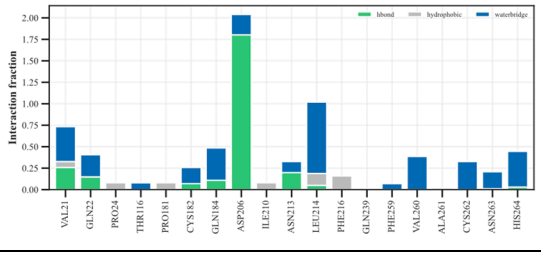
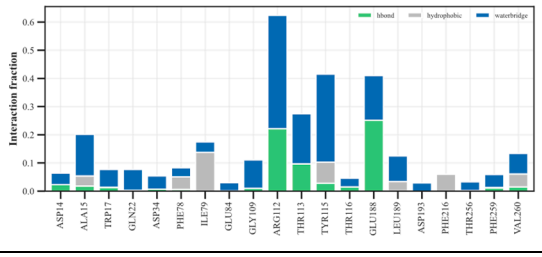
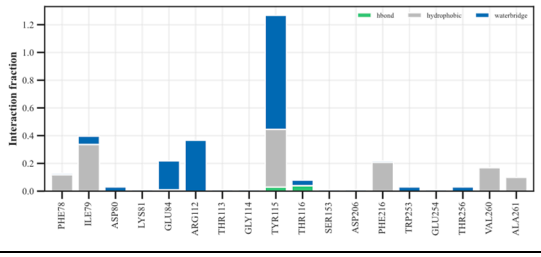
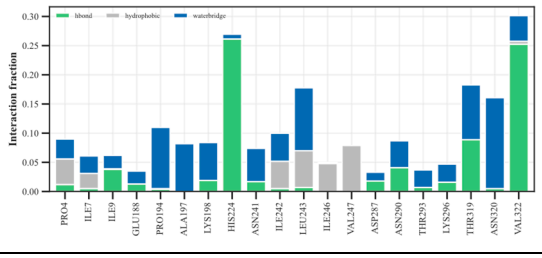
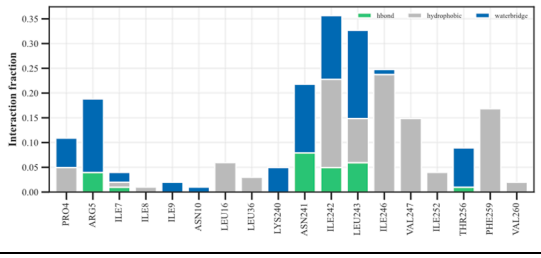
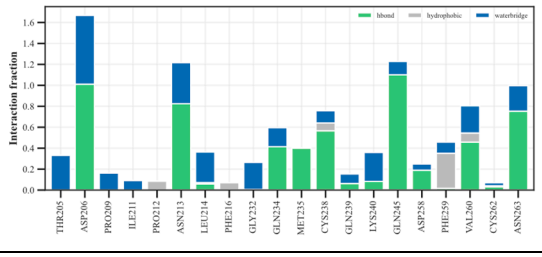
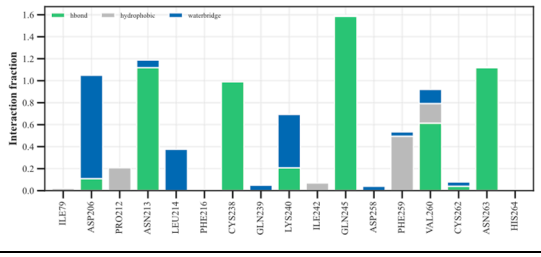
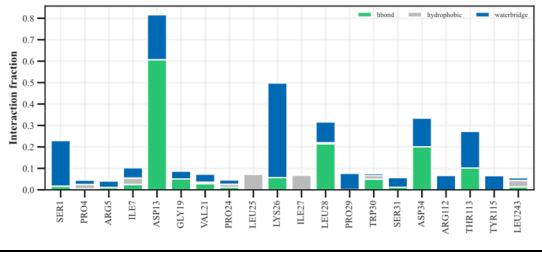
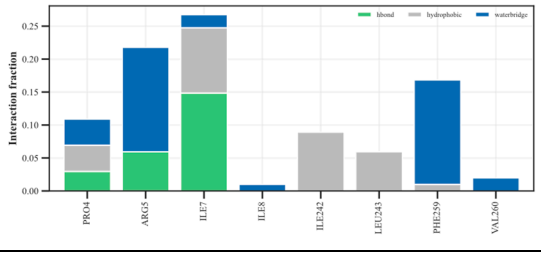
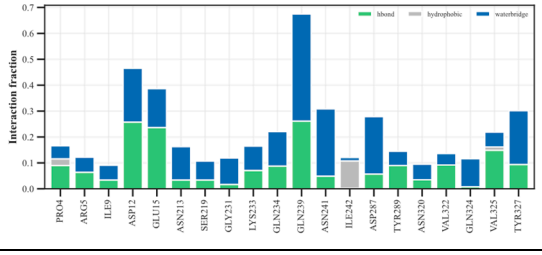
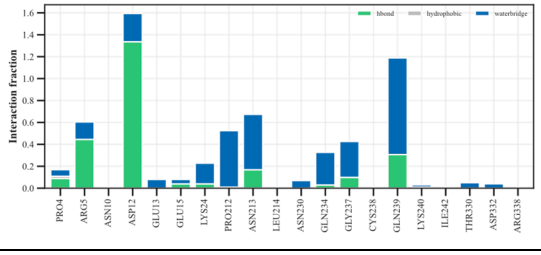
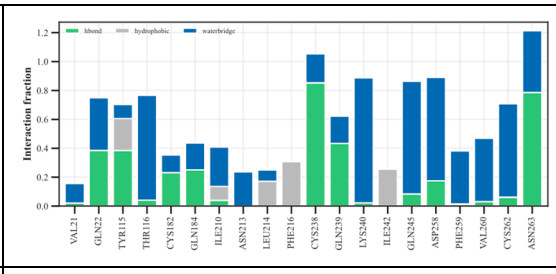
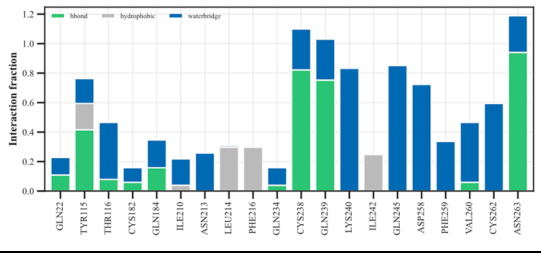
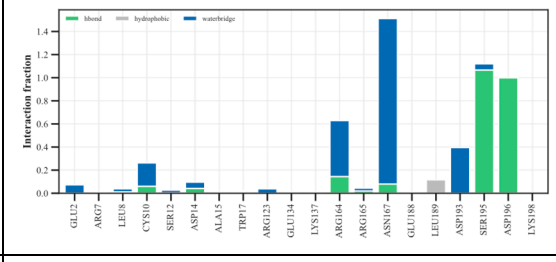
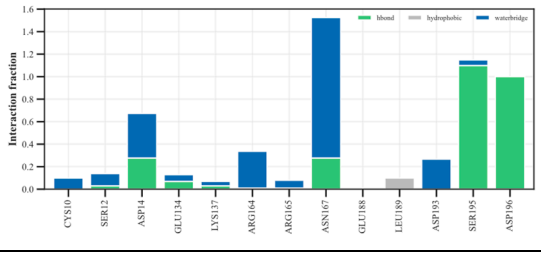
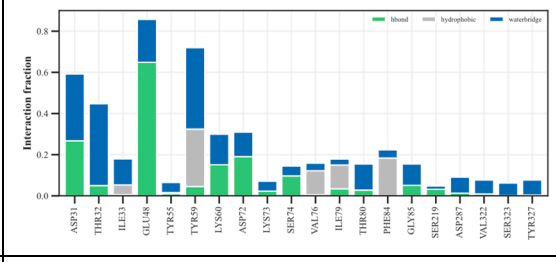
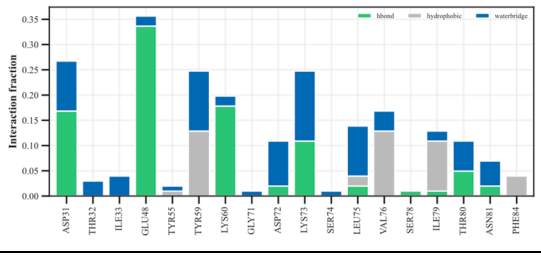
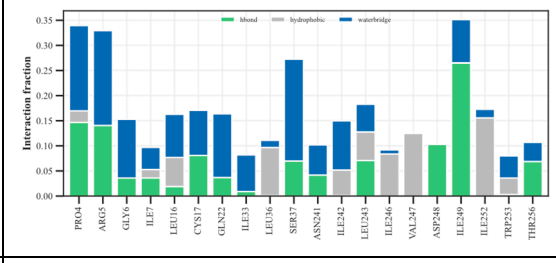
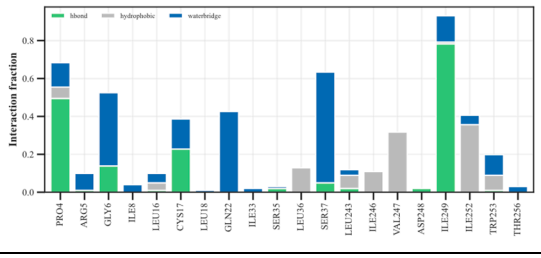
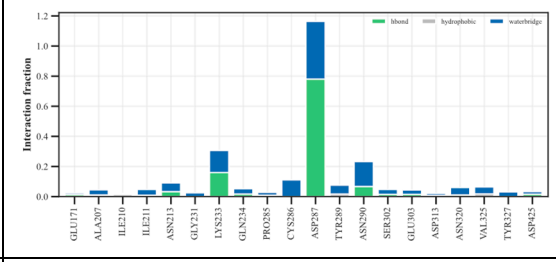
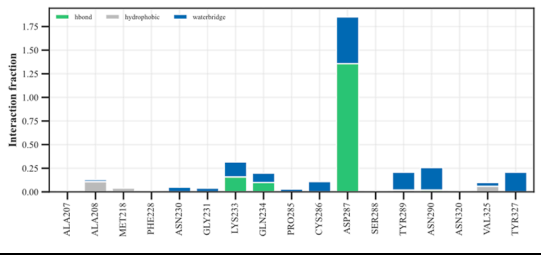
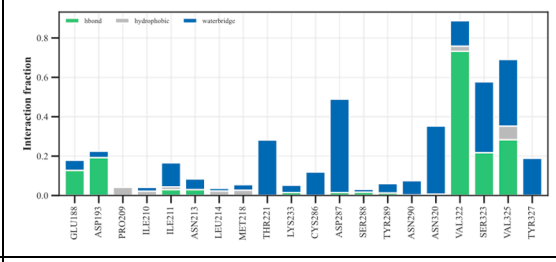
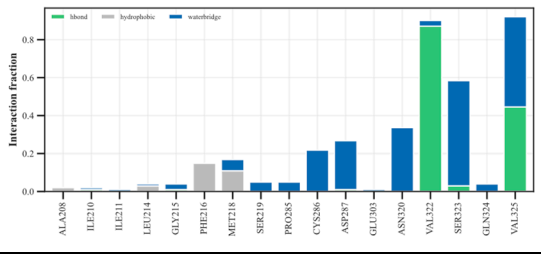
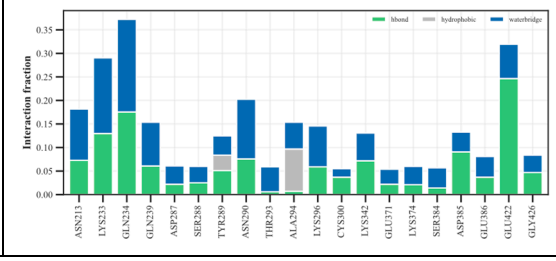
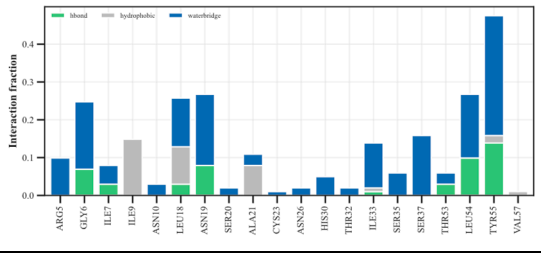
Herniariasaponin 2	
Herniariasaponin 4	

Figure S3. Ligand-protein contacts were formed throughout the entire 500 ns molecular dynamics simulation and during the last 50 ns.

Ligand	Contacts (Full Trajectory)	Contacts (Last 50 ns)
Cholate (Site 1)		
Cholate (Site 2)		
Cholate (Site 3)		

Escin Ia (Site 1)		
Escin Ia (Site 2)		
Escin Ia (Site 3)		
Hederacoside C (Site 1)		
Hederacoside C (Site 2)		
Hederacoside C (Site 3)		
Ginsenoside Rb1 (Site 1)		

Ginsenoside Rb1 (Site 2)		
Ginsenoside Rb1 (Site 3)		
Ginsenoside Re (Site 1)		
Ginsenoside Re (Site 2)		
Ginsenoside Re (Site 3)		
Ginsenoside Rd (Site 1)		
Ginsenoside Rd (Site 2)		

Ginsenoside Rd (Site 3)		
Ginsenoside Rg1 (Site 1)		
Ginsenoside Rg1 (Site 2)		
Ginsenoside Rg1 (Site 3)		
Osladin (Site 1)		
Osladin (Site 2)		
Osladin (Site 3)		

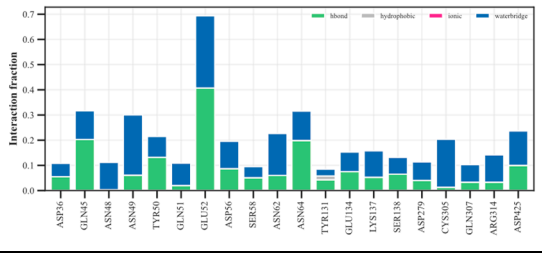
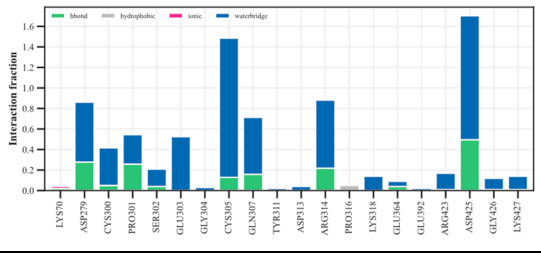
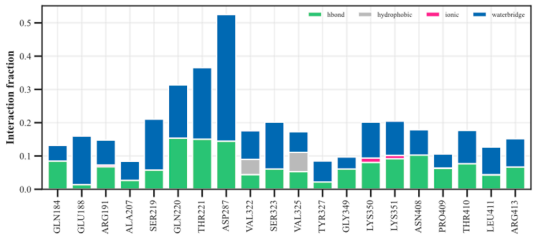
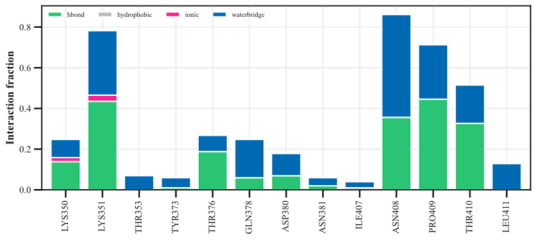
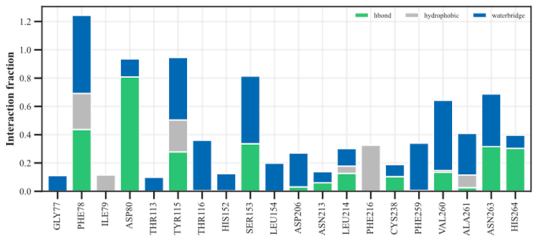
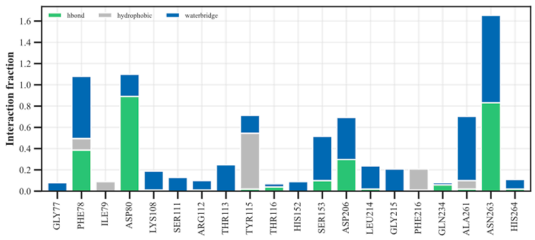
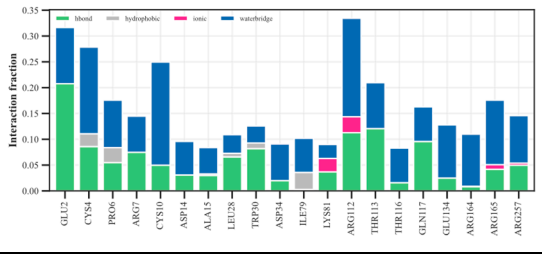
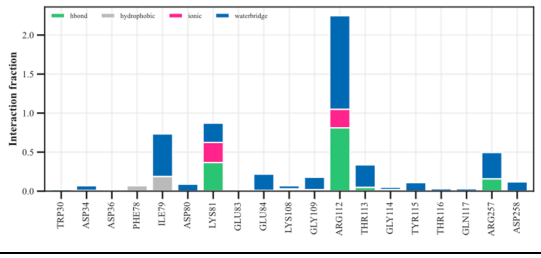
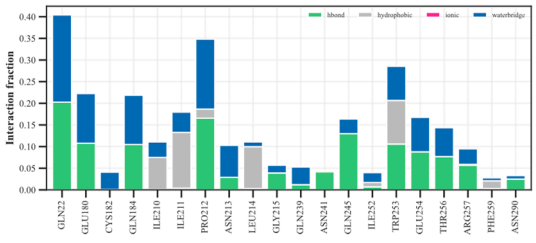
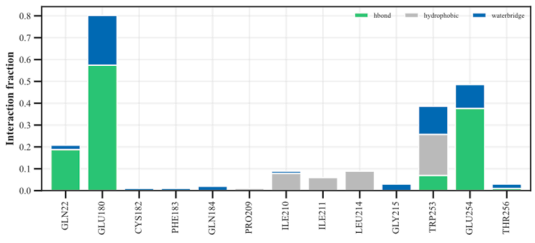
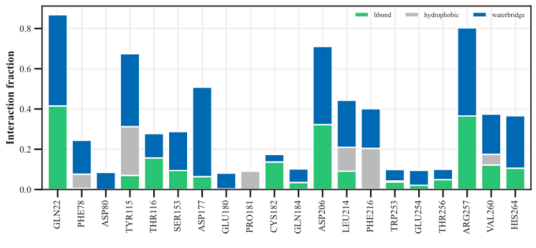
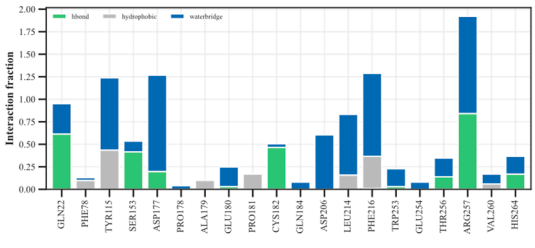
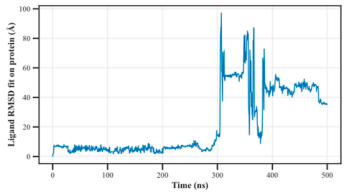
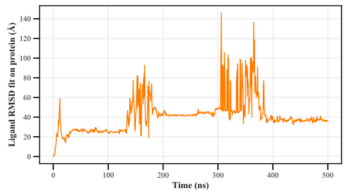
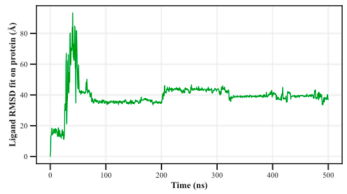
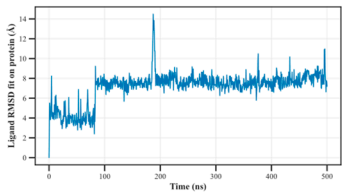
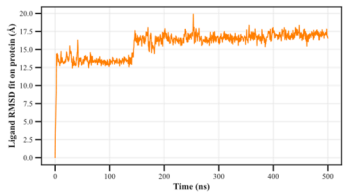
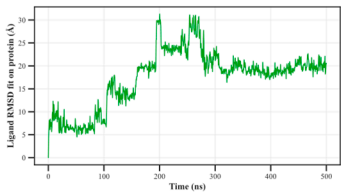
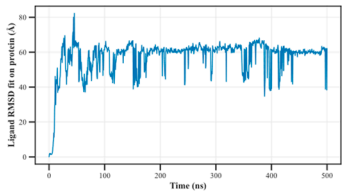
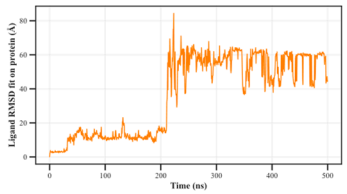
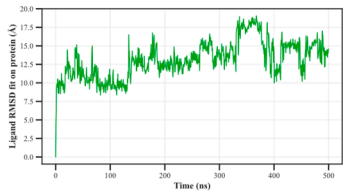
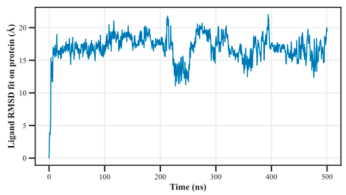
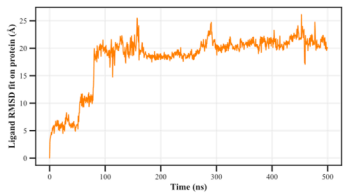
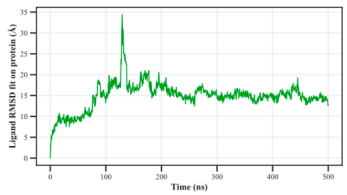
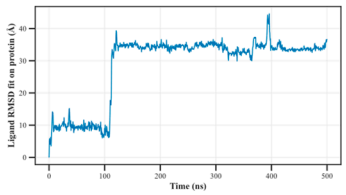
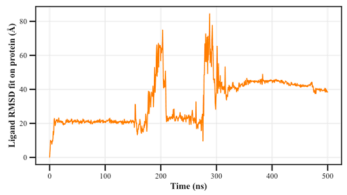
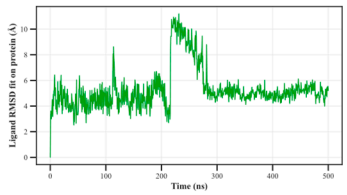
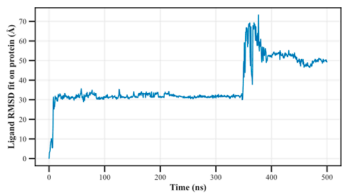
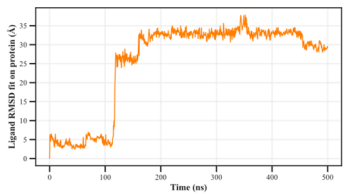
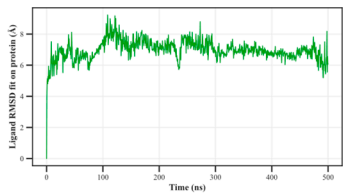
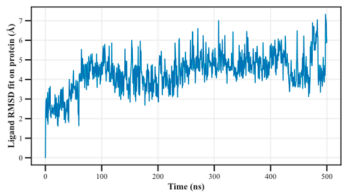
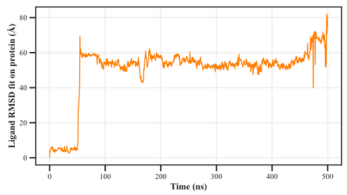
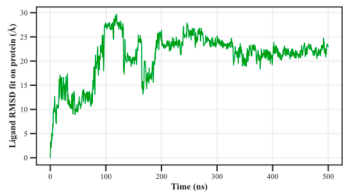
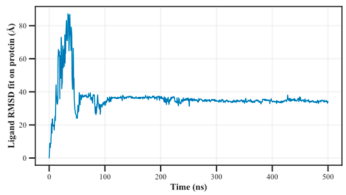
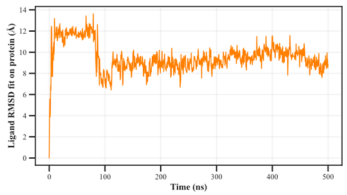
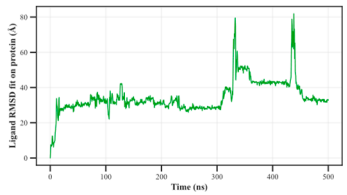
Herniariasaponin 2 (Site 1)		
Herniariasaponin 2 (Site 2)		
Herniariasaponin 2 (Site 3)		
Herniariasaponin 4 (Site 1)		
Herniariasaponin 4 (Site 2)		
Herniariasaponin 4 (Site 3)		

Figure S4. Ligand Root Mean Square Deviation (RMSD) values throughout a 500 ns molecular dynamics simulation for saponin-lipase-colipase complexes.

Ligand	RMSD (site 1)	RMSD (site 2)	RMSD (site 3)
Cholate			
Escin Ia			
Hederacoside			
Ginsenoside Rb1			
Ginsenoside Re			
Ginsenoside Rd			
Ginsenoside Rg1			
Osladin			

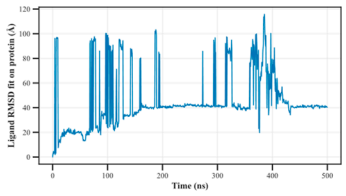
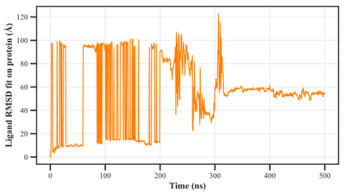
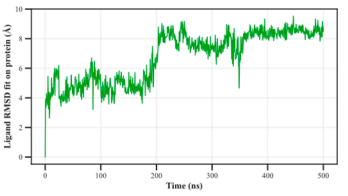
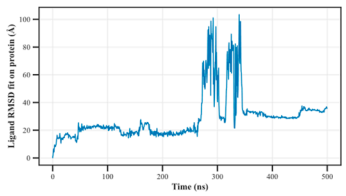
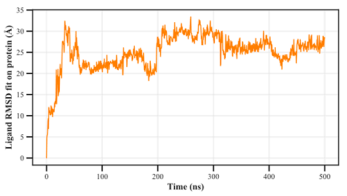
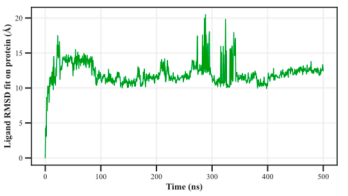
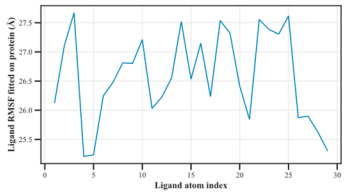
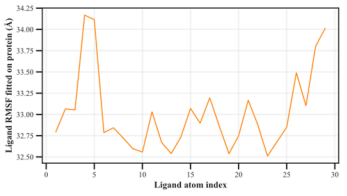
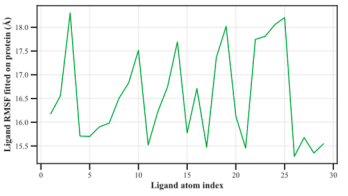
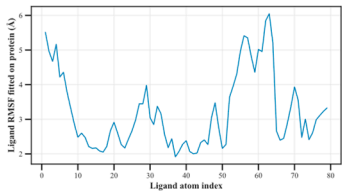
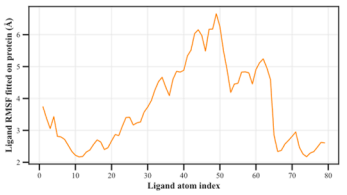
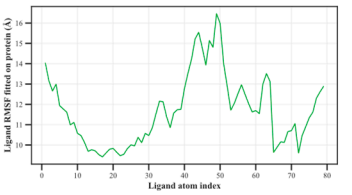
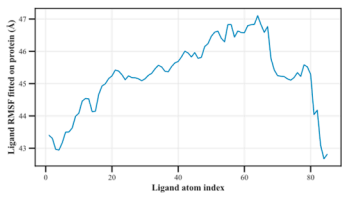
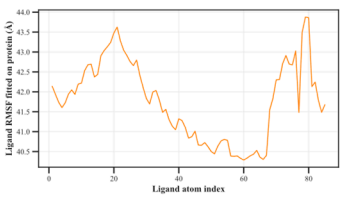
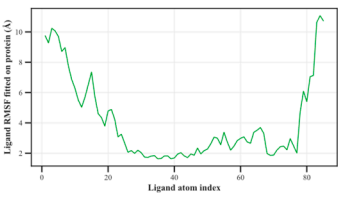
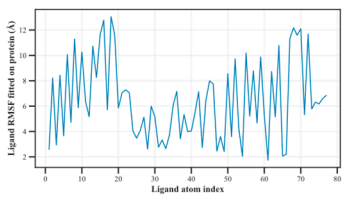
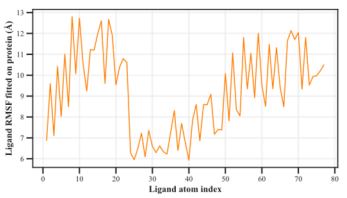
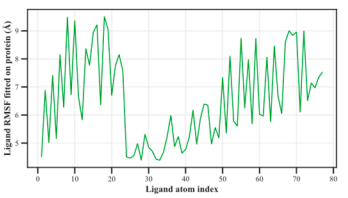
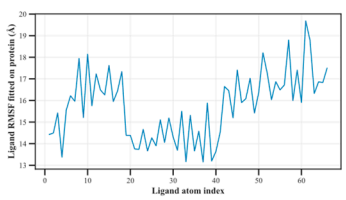
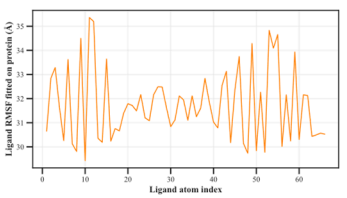
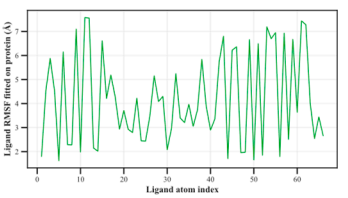
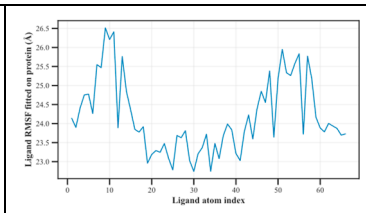
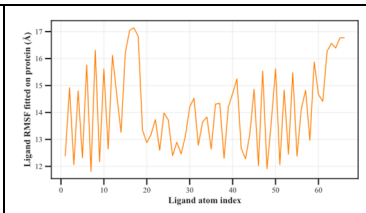
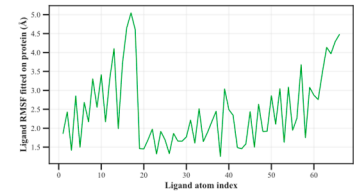
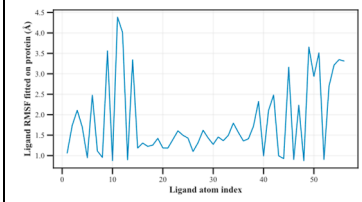
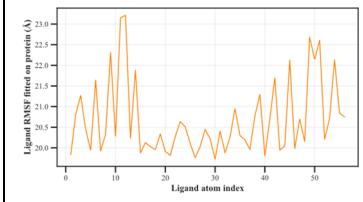
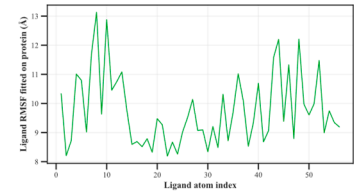
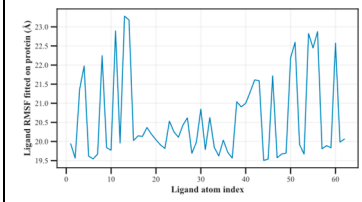
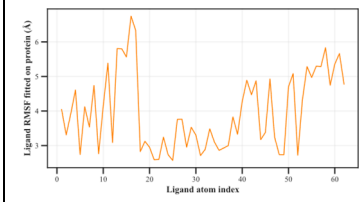
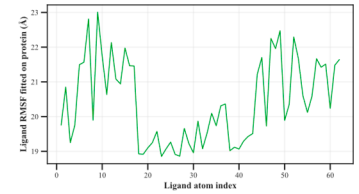
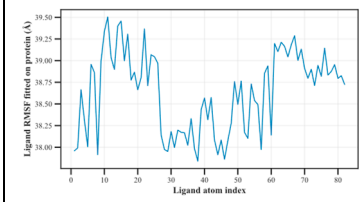
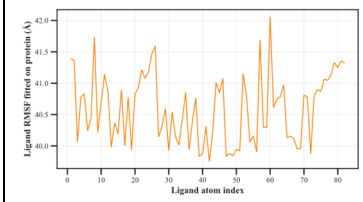
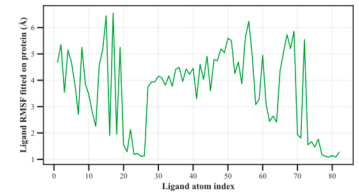
Herniariasaponin 2			
Herniariasaponin 4			

Figure S5. Ligand Root Mean Square Fluctuation (RMSF) values throughout a 500 ns molecular dynamics simulation for saponin-lipase-colipase complexes.

Ligand	RMSF (site 1)	RMSF (site 2)	RMSF (site 3)
Cholate			
Escin Ia			
Hederacoside			
Ginsenoside Rb1			
Ginsenoside Re			

Ginsenoside Rd			
Ginsenoside Rg1			
Osladin			
Herniariasaponin 2			
Herniariasaponin 4	