Supplementary Materials:

Virtual Screening Using Pharmacophore Models Retrieved From Molecular Dynamic Simulations

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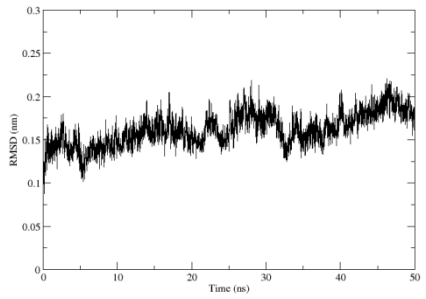
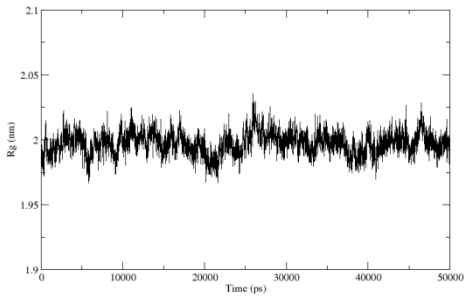
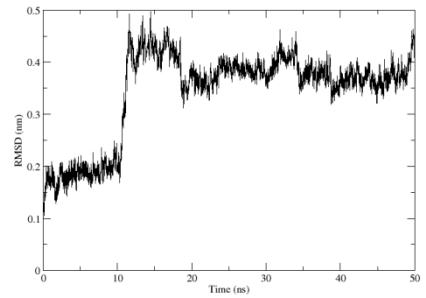
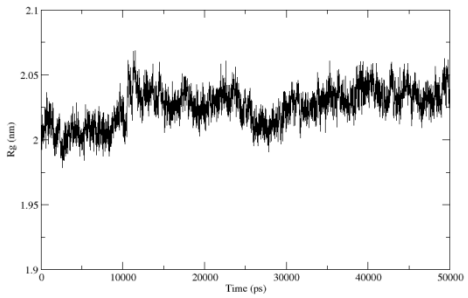
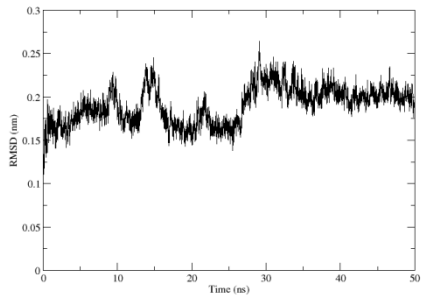
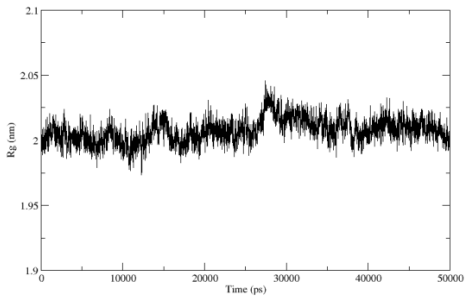
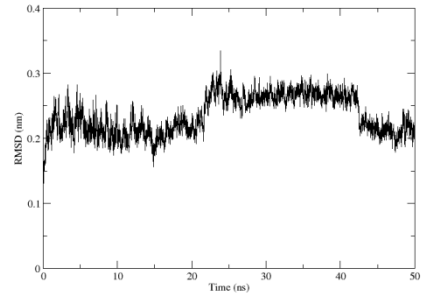
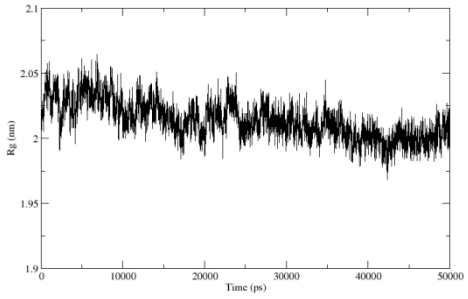
PDB code	RMSD plot (compared with initial structure after least square fit to backbone)	Radius of gyration
2C6O		
2FVD		
2XMY		
5D1J		

Figure S1. RMSD and radius of gyration plots from MD simulation of four studied complexes.

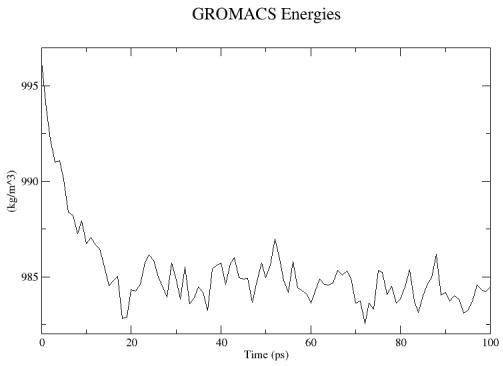
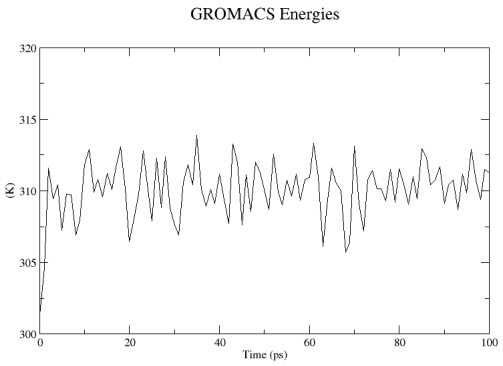
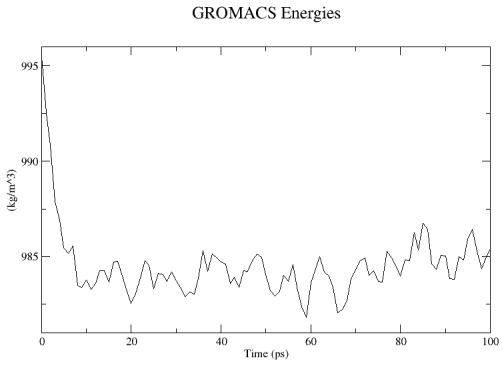
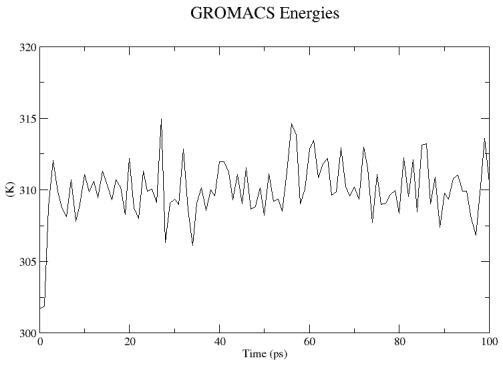
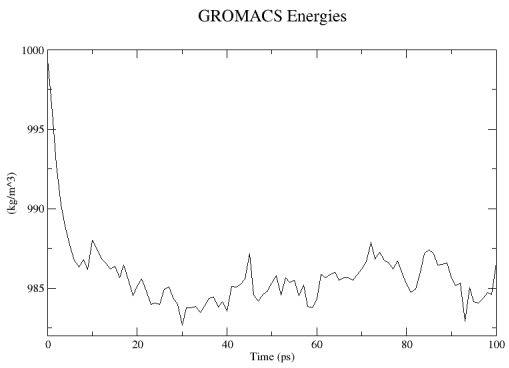
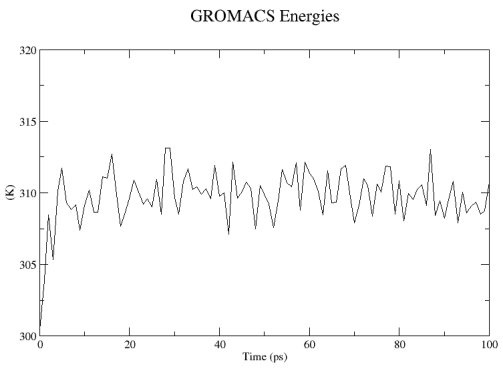
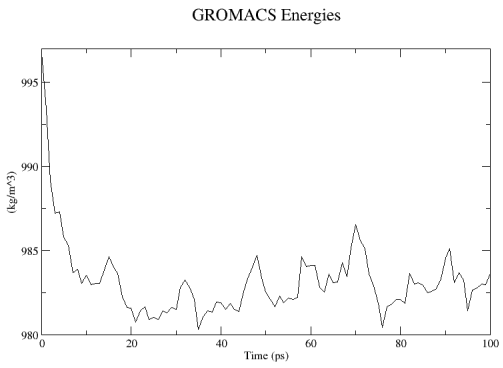
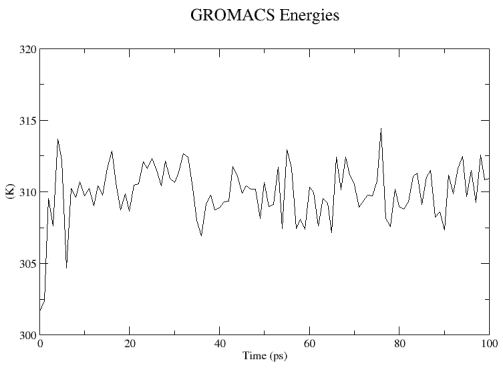
PDB code	Density	Temperature
2C6O		
2FVD		
2XMY		
5D1J		

Figure S2. Density and temperature plot during the equilibration stage of MD simulations of four studied complexes.

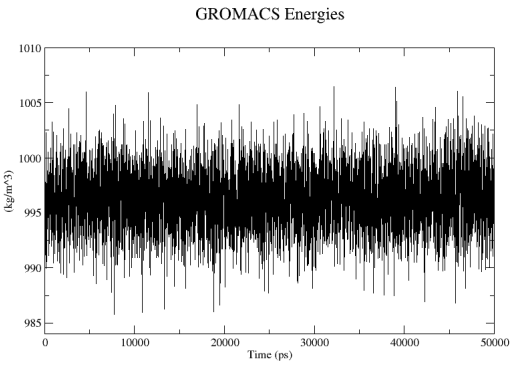
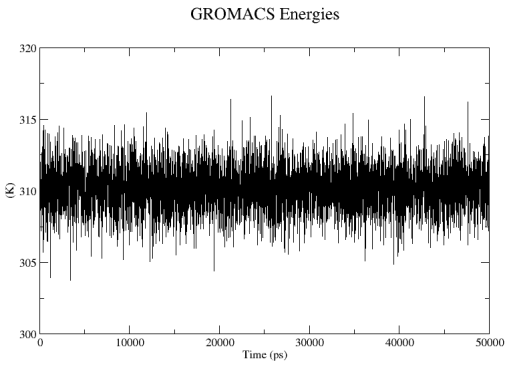
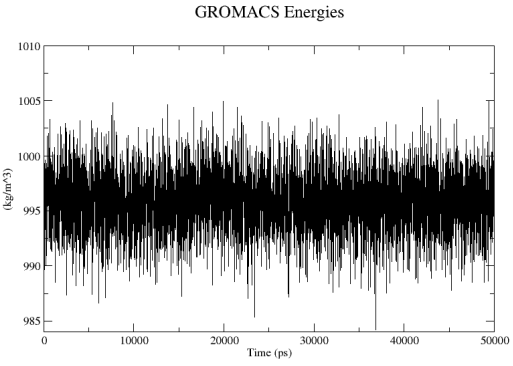
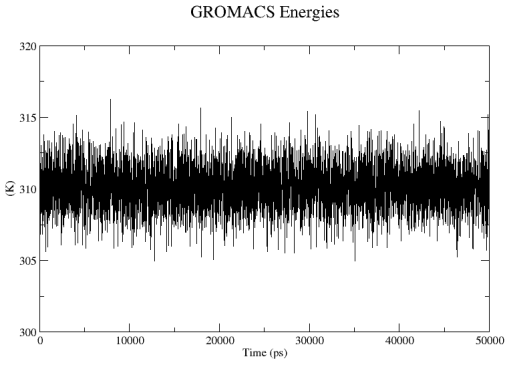
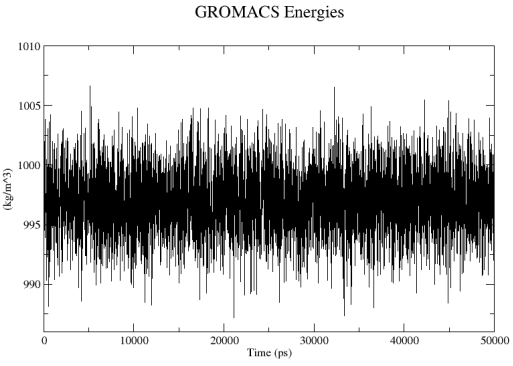
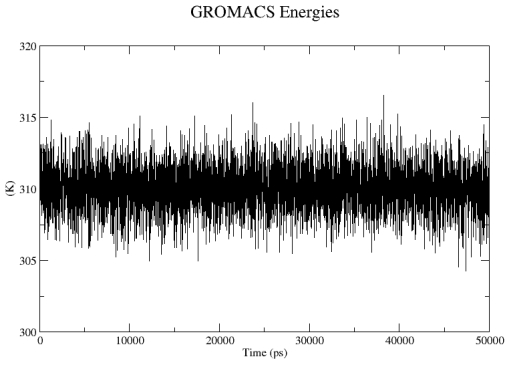
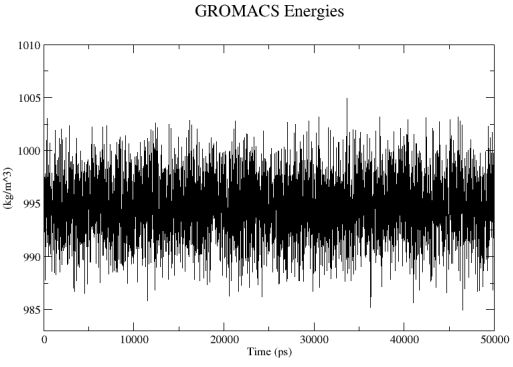
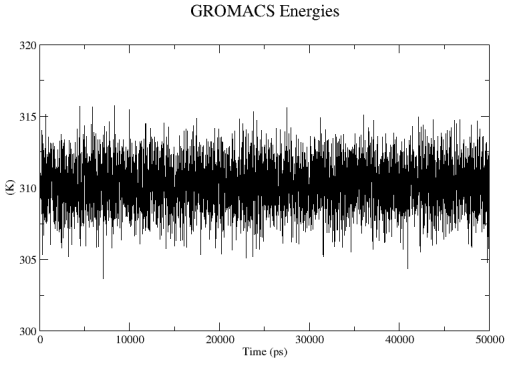
PDB code	Density	Temperature
2C6O		
2FVD		
2XMY		
5D1J		

Figure S3. Density and temperature plot during the production stage of MD simulations of four studied complexes.