



Fig. S1 RMSD of PPO systems during the pressurization and depressurization stages from MD simulations. RMSD plots of 0.1 MPa, under 100 MPa, under 300MPa, and under 500MPa (a); 0.1 MPa, after 100 MPa, after 300 MPa, after 500 MPa (b). RMSD Histograms of 0.1 MPa, under 100 MPa, under 300MPa, and under 500MPa (c); 0.1 MPa, after 100 MPa, after 300 MPa, after 500 MPa (d).