

1 **Video 1.** A molecular dynamics simulation shows electrostatic interactions between suramin molecules (stick
2 representation) and the histone octamer (cartoon representation), with hidden water molecules and counter ions for
3 clarity. Six suramin molecules were first arbitrarily placed in the simulation box at the proximity of histone. At the
4 end of the 700-ns simulation, five of six suramin molecules formed stable contacts with the protein, mainly via salt
5 bridges and hydrogen bonding.