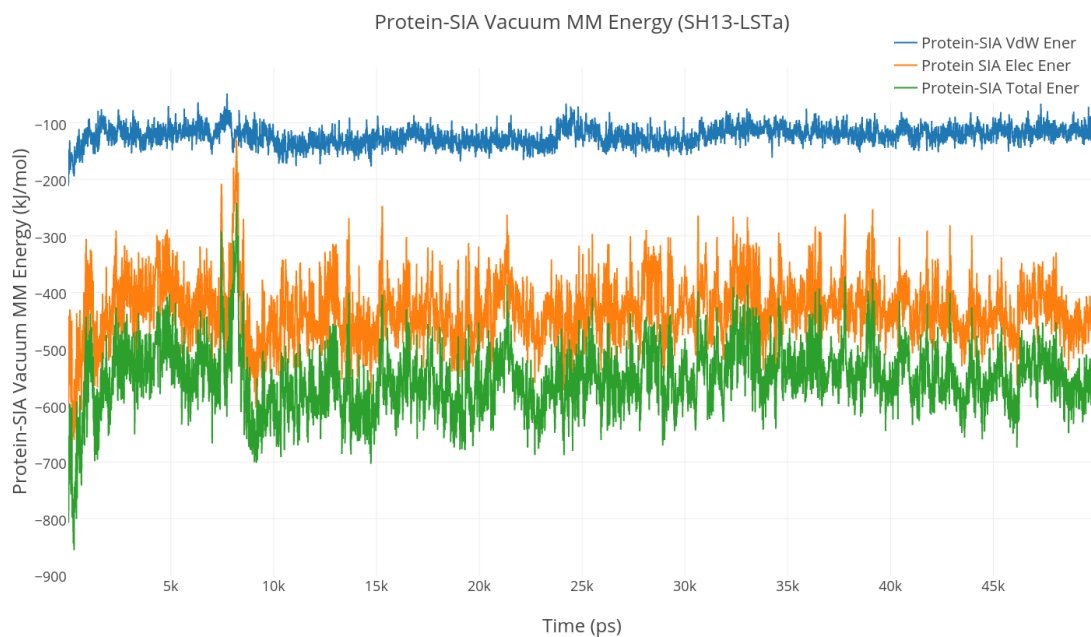


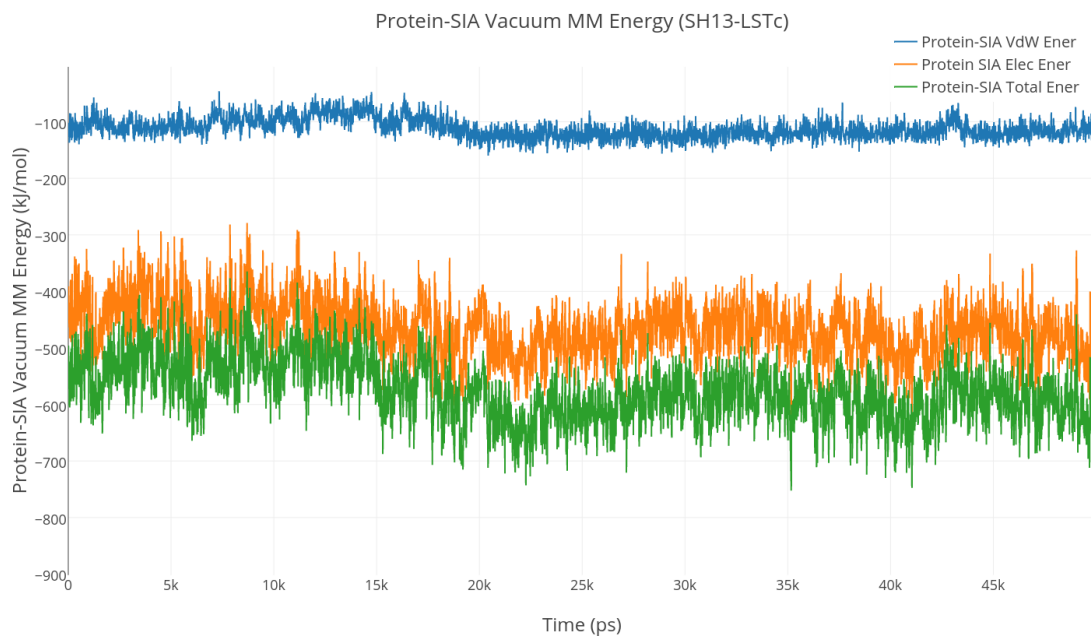
Additional file 3. VdW energy, electrostatic energy and total interaction energy of SH13-LSTa, SH13-LSTc, TW17-LSTa and TW17-LSTc during the whole simulation (50 ns).

The total energy of TW17-LSTa fluctuated obviously during around 25 ns. Each trajectory fluctuated within a small range after 30ns. Therefore, we chose the last 20 ns frames for further analysis.

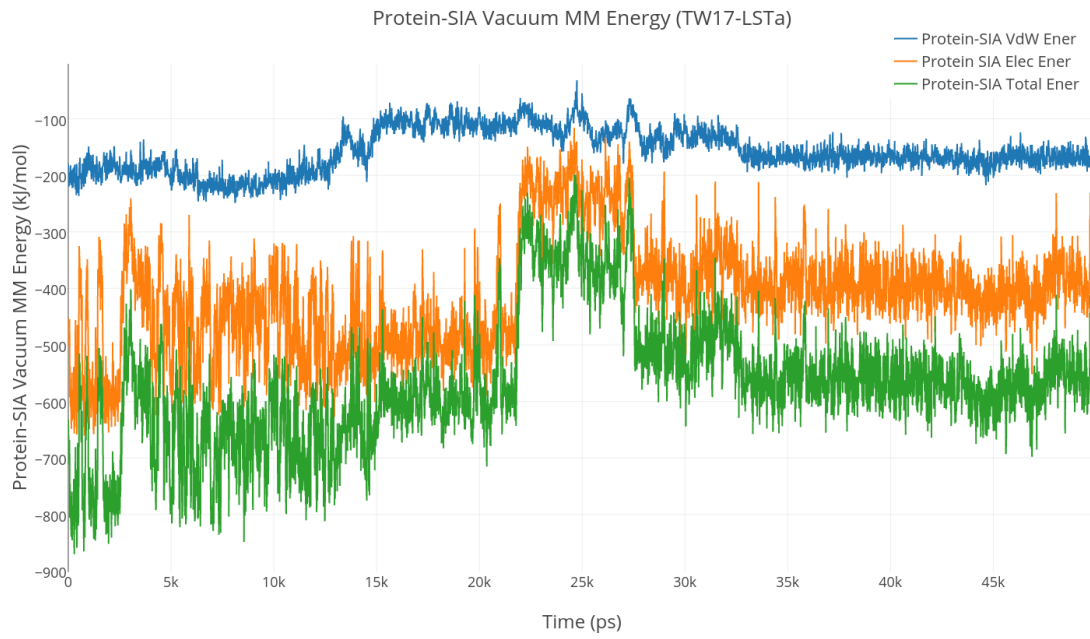
1. SH13-LSTa



2. SH13-LSTc



3. TW17-LSTa



4. TW17-LSTc

