VdW non-bonded energies (Elec+VdW) -500 -500 · -550 -550 --600 -600 -2000 1500 1000 500 1000 2000 -500 **-**-500 **-**-550 -Energy (kcal/mol) -600 **-**-650 -700 **-**2000 500 1000 1500 500 1000 1500 2000 sw22 sw25 -500 **-**-500 · -550 · -550 -600 --700 **-**-700 **-**500 1000 1500 500 1000 1500 2000 TIME (x5000fs)