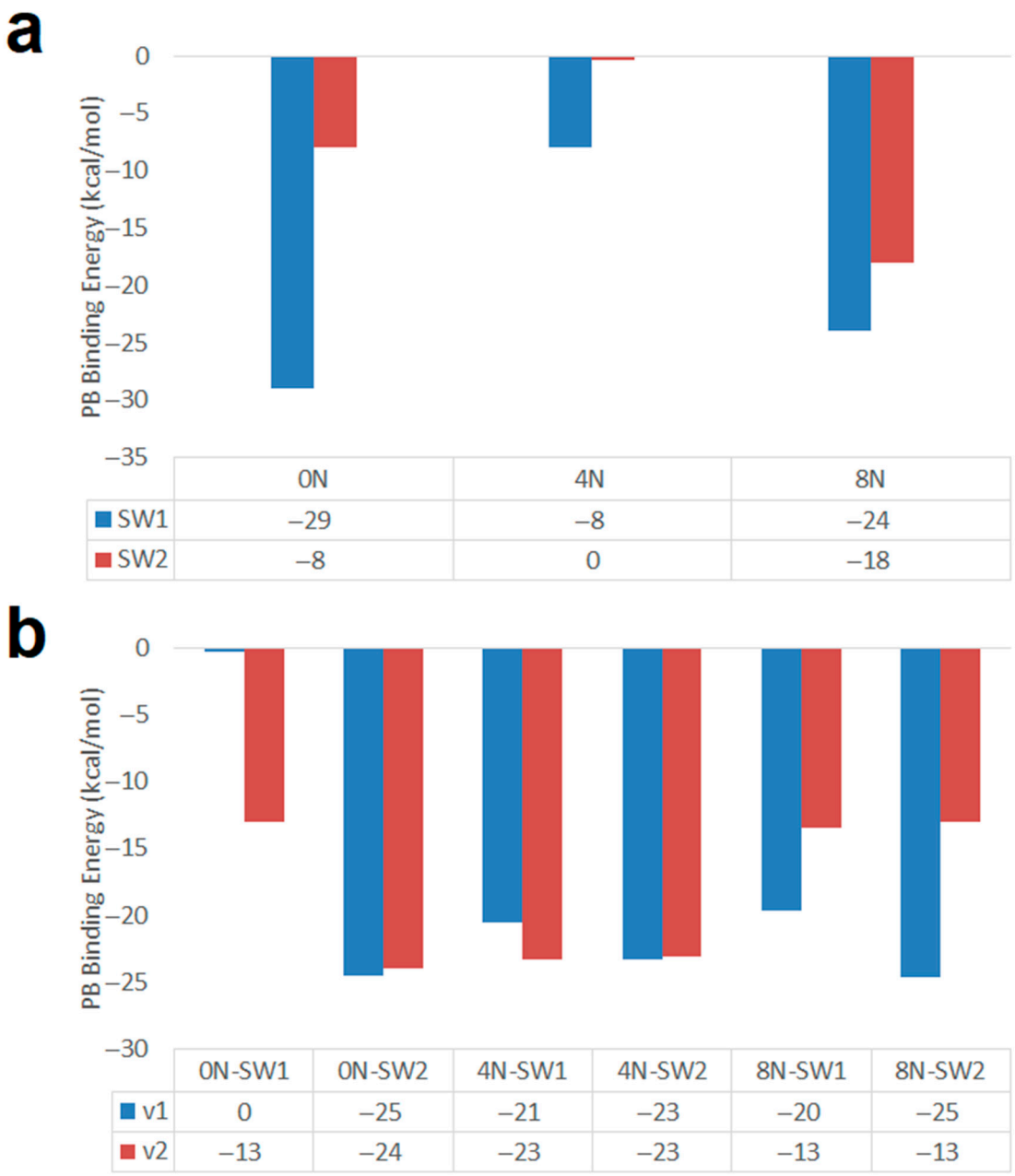

Figure S1. DOX-CNT PB relative binding energies for nitrogen-doped and undoped (10,10) *armchair* nanotubes of different length having one and two Stone-Wales defects. (a) 20 Å length; reference: 4N doped SW2 nanotube with –110 kcal/mol PB DOX-CNT binding energy; (b) 34 Å length; reference: 0N SW1 nanotube with –105 kcal/mol PB DOX-CNT binding energy.

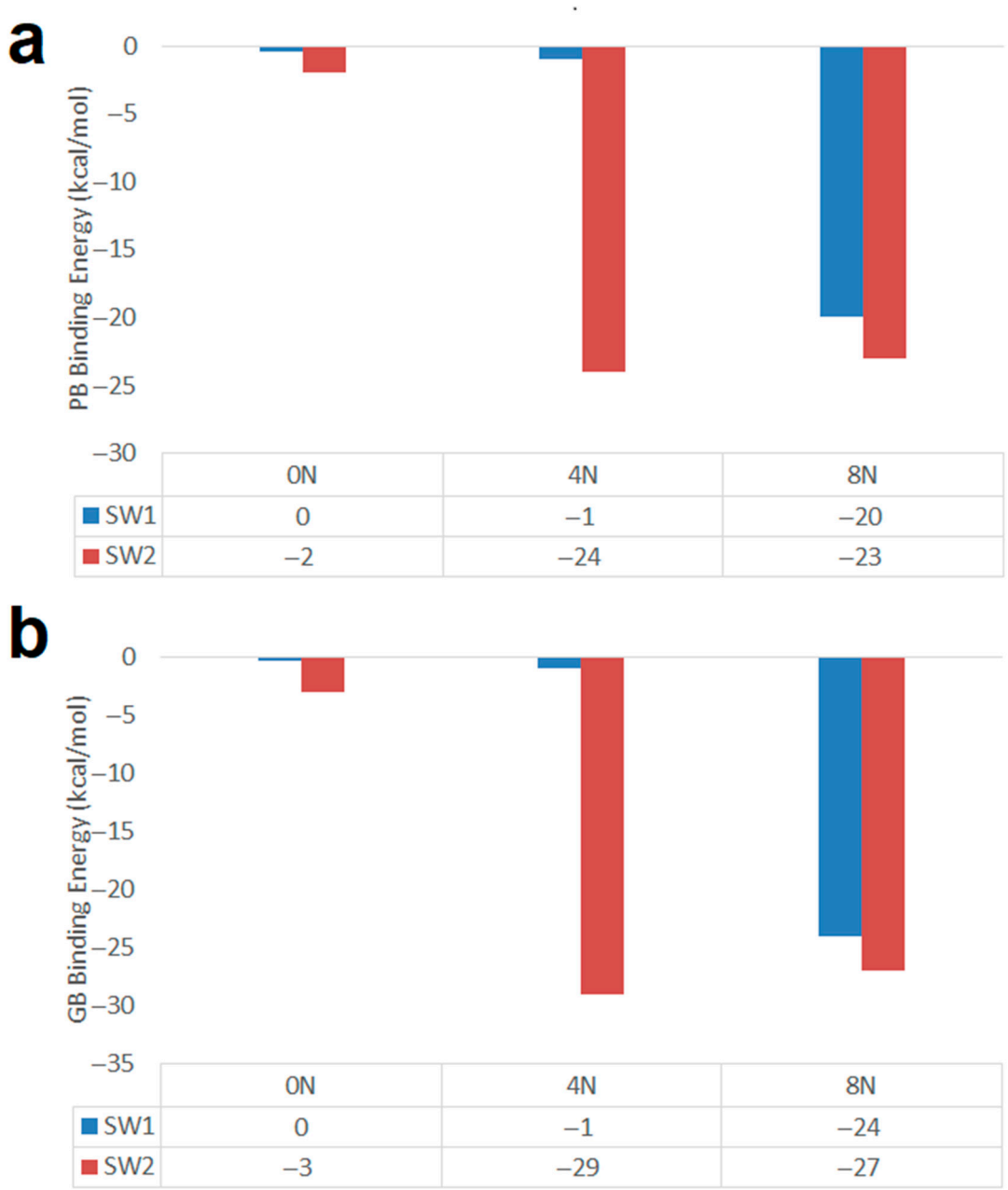

Figure S2. Representation of the PB and GB DOX-CNT relative binding energies for nitrogen-doped and undoped (18,0) *zigzag* nanotubes having one and two Stone-Wales defects. (a) PB binding energy. Reference: 0N SW1 nanotube with –102 kcal/mol PB DOX-CNT binding energy; (b) GB binding energy. Reference: 0N SW1 nanotube with –107 kcal/mol GB DOX-CNT binding energy.