Supporting Information

Binding Preference of Carbon Nanotube Over Proline-Rich Motif Ligand on SH3-domain: A Comparison with Different Force Fields

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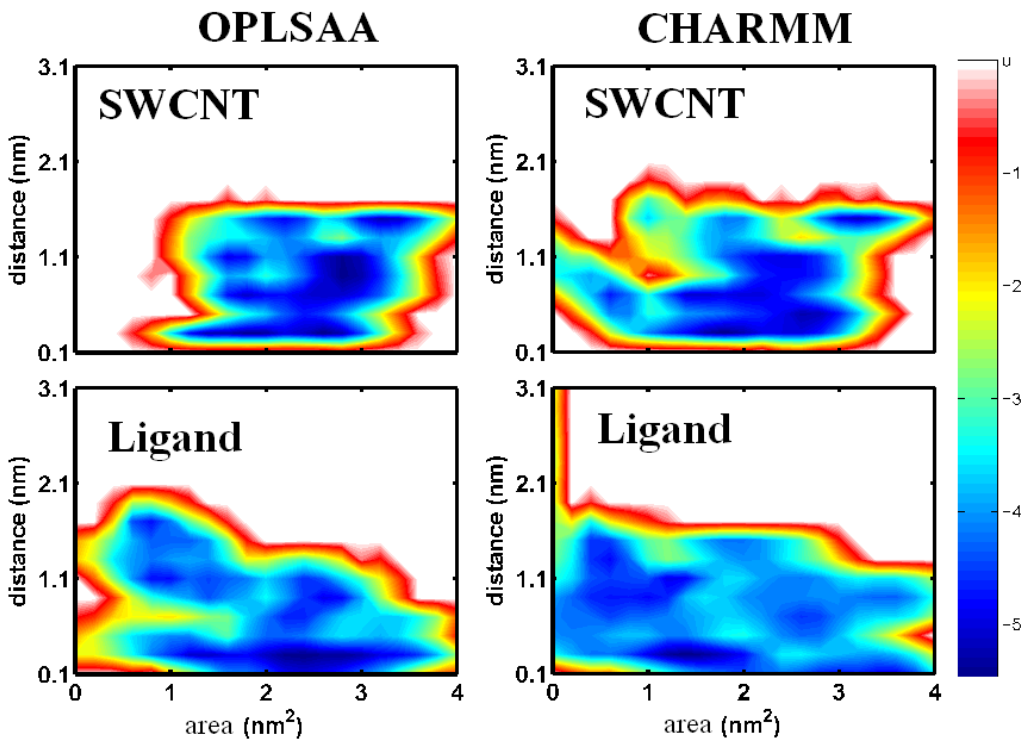

Fig. S1 Binding free energy landscapes of the SWCNT (top two) and the ligand (bottom two) with the SH3 domain. The area denotes the interface area of the SWCNT and ligand with the SH3 domain, respectively. The distance is the minimal distance of the SWCNT and the ligand from these key residues, respectively. The unit of the free energy is kcal/mol.