Electronic Supporting Information.

Detailed description of movies: Movie_1: Initial tube (14,0), the same tube and tube (14,0) modified, addition of phenol to last two boxes, tubes with added water (water inside marked in blue), kinetics of mixing (note that phenol is not adsorbed in the modified tube and pumps out water from the initial tube). The last few frames show equilibrium situation after 6 ns. Movie_2: First row – initial tubes (8,0) and (26,0), second rows – modified tubes, two of the three studied adsorbates: phenol and paracetamol, equilibrated configurations (solvent not shown for clarity) adsorbed molecules form spiral structures wrapping nanotubes. Movie_3: Initial (14,0) tubes, the same tubes with benzene, phenol and paracetamol and water, kinetics of the pumping effect – bottom panel shows the situation on external surface of CN.

Simulation methodology and calculations: MD simulations were performed using the Groningen Machine for Chemical Simulation (GROMACS) v.3.2.1 [S1]. The studied molecules were modelled in the OPLSAA force field [S2-S4] (projected for simulation of condensed phases) and we obtained excellent reproducibility of the bulk properties of all studied adsorbents (i.e. densities, melting and boiling point temperatures, molar volumes, RDFs, etc.). The charges of atoms forming the phenol molecule were taken from Mooney et al. [S5]. For paracetamol molecules they were calculated using the DFT method B3LYP functional and basis set (b3lyp/6-31g(d,p)) implemented in the Gaussian 03 quantum chemical package [S6]. For benzene they were taken from the paper of Jorgensen and Severance [S7]. Water was simulated using the TIP4P model [S8]. All simulations were performed for the temperature of 298.15 K in cubicoid boxes with dimensions proportional to the tube dimensions (the number of water molecules ranged from c.a. 3000 for (8,0) up to 7000 for (26,0) tube). We also repeated simulations for tubes (14,0) and (20,0) in boxes with longer z dimension (along axis) and we obtain the same results. Carbon nanotubes (from (8,0)

up to (26,0)) contain 624, 1092, 1560 and 2028 carbon atoms, oxidized nanotubes contain additionally 16, 28, 40 and 52 oxygen atoms. Tubes were rigid during simulations. Surface oxygen groups were introduced by a "virtual oxidation" process i.e. all carbon atoms at the edge of SWCN were saturated by oxygen forming carbonyls. The charges of carbon and oxygen were equal to +0.5 and -0.5, respectively. Simulations were performed in the Canonical Ensemble with Berendsen thermostat (the density of water far from the tube after simulations is always 0.987 g/cm^3). Periodic boundary conditions were applied in all three directions, PME method was applied for calculation of the electrostatic interactions, and the number of solute molecules was 50 per box. The parameters for carbon were adopted from [S9, S10]. Simulations were performed for the time range 6000 ps. To ensure that the full equilibrium exists the kinetic, potential and the ration of kinetic/potential energies were calculated. We also constructed the program calculating the number of water and adsorbate molecules inside and outside tubes and the kinetic curves show that equilibrium was reached. All reported final results were obtained as the average from last 500 ps. To determine the average orientation between the benzene ring plane of studied molecules and the plane perpendicular to the radius of the tube passing the centre of the benzene ring (this is equivalent to the angle between the plane of the benzene ring and the plane tangential to the tube) we consider only the molecules inside the tube or being in contact with the external surface. We assumed the distance between the centre of the ring and the axis of the tube was not larger than the tube radius plus 0.7 nm. Density profiles were determined assuming that the centre of the molecules is located at the centre of benzene ring, and for water molecules this centre is located on oxygen atom. Calculated in this way density is the averaged (also from last 500 ps) ratio of the number of points determining the orientation of a given molecule in the volume element per volume. This density was studied as a function of the distance from the tube axis (r) and the z axis (the direction of the tube axis). The simulation

box was divided in z direction on 50 layers, and for the distance from the tube axis on 100 layers (maximum distance from the tube axis corresponds a half of the smaller dimension of the box along x or y axis). The statistics of hydrogen bonds was calculated using the method described by Gordillo and Marti [22]. The results were obtained as the average number hydrogen bonds produced by one water molecule as a function of the distance from the axis of the tube. As molecules located inside tubes were considered those having z coordinates of oxygen atom placed between the z coordinates of the terminal tube carbon (initial tubes) or oxygen (modified tubes) atoms.

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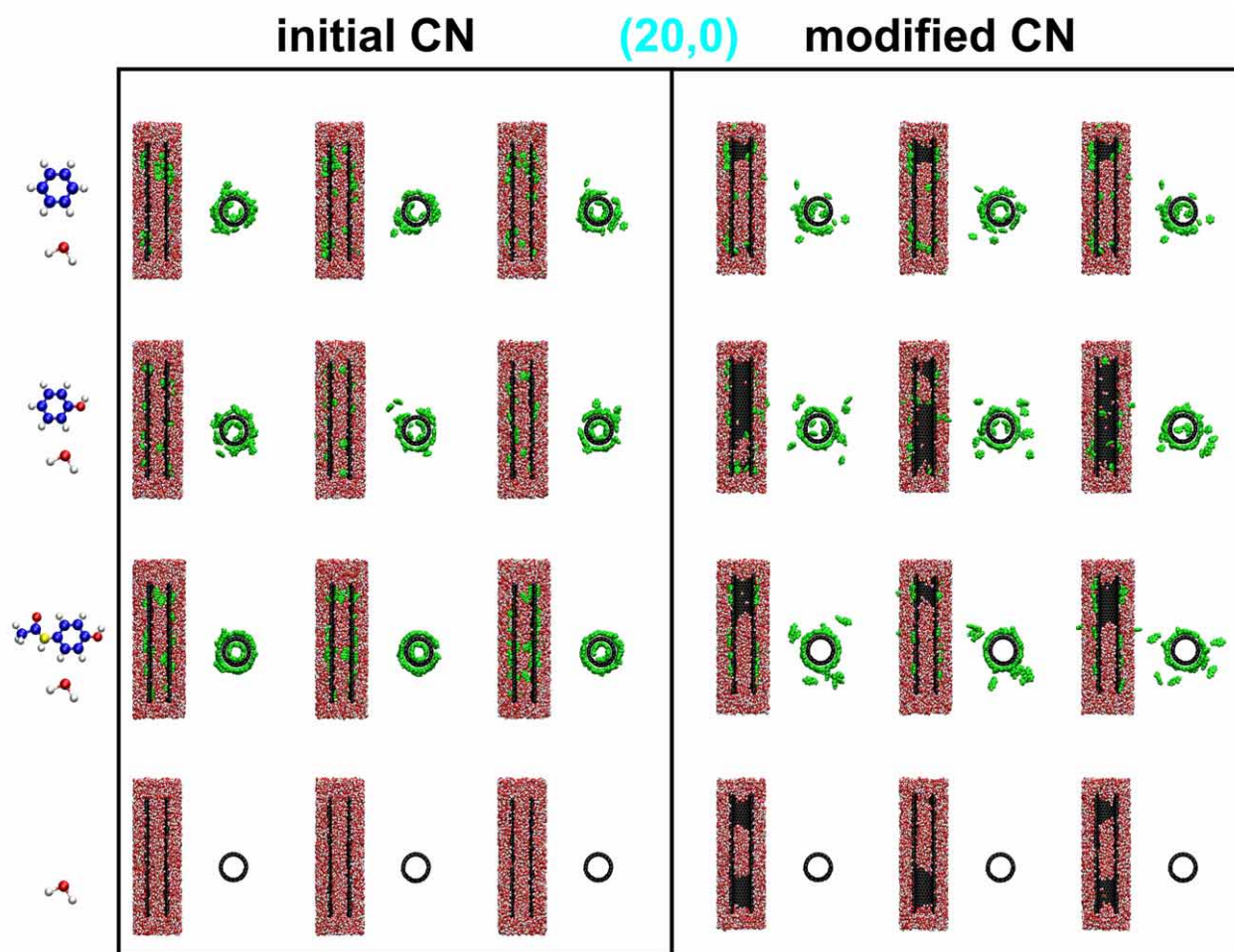
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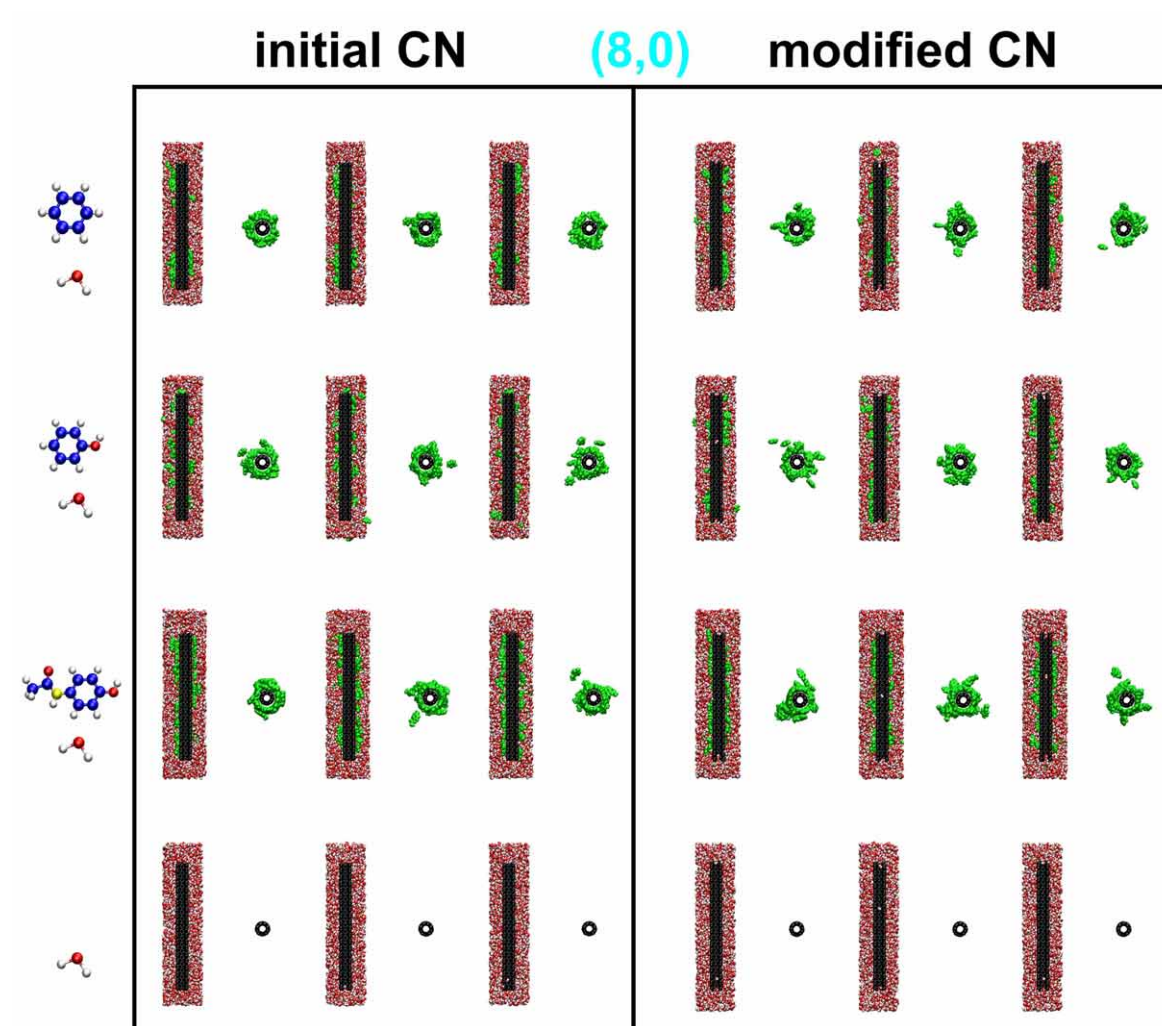
Figure S1. Equilibrium configurations for studied adsorbates, water and tubes (8,0).
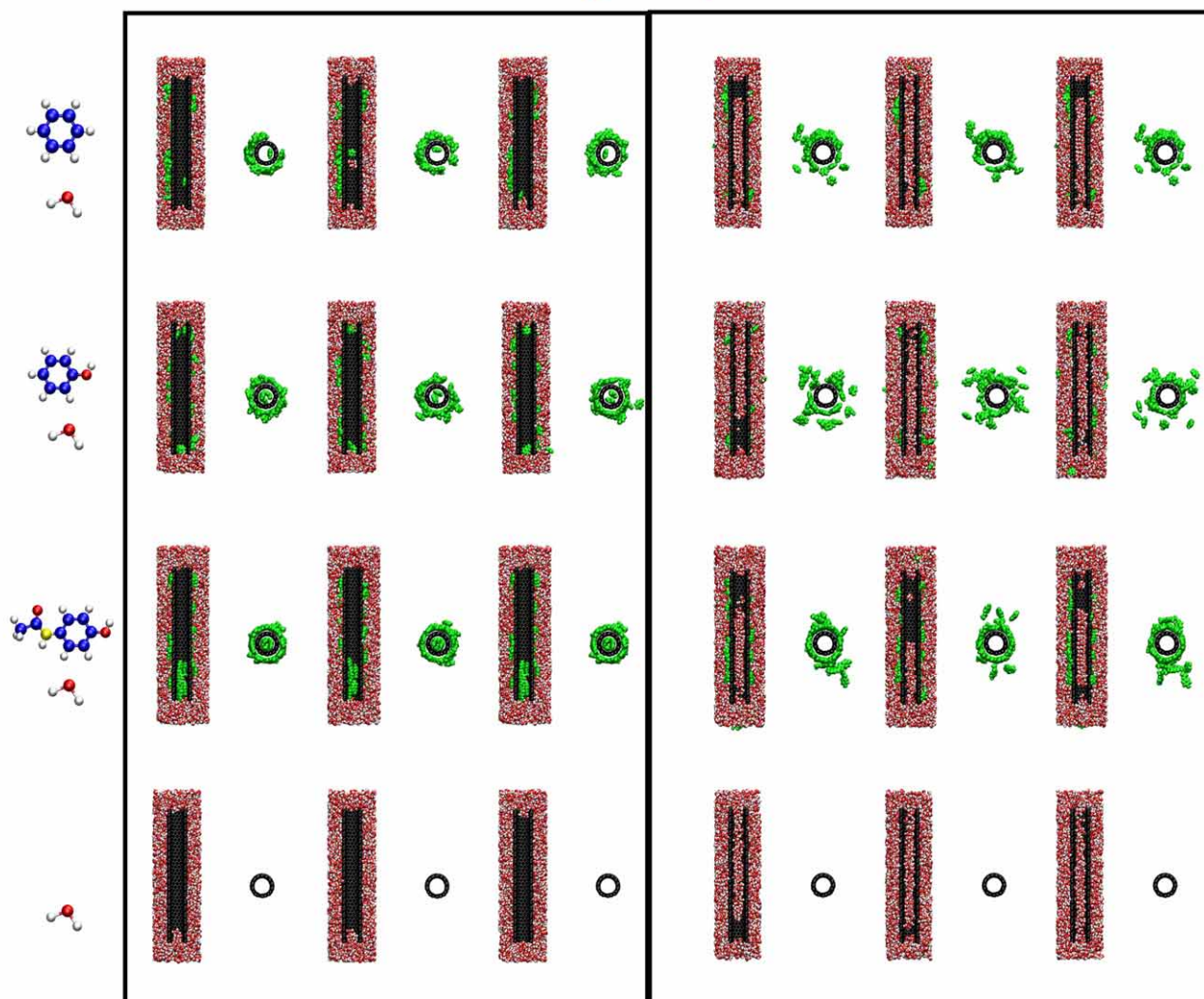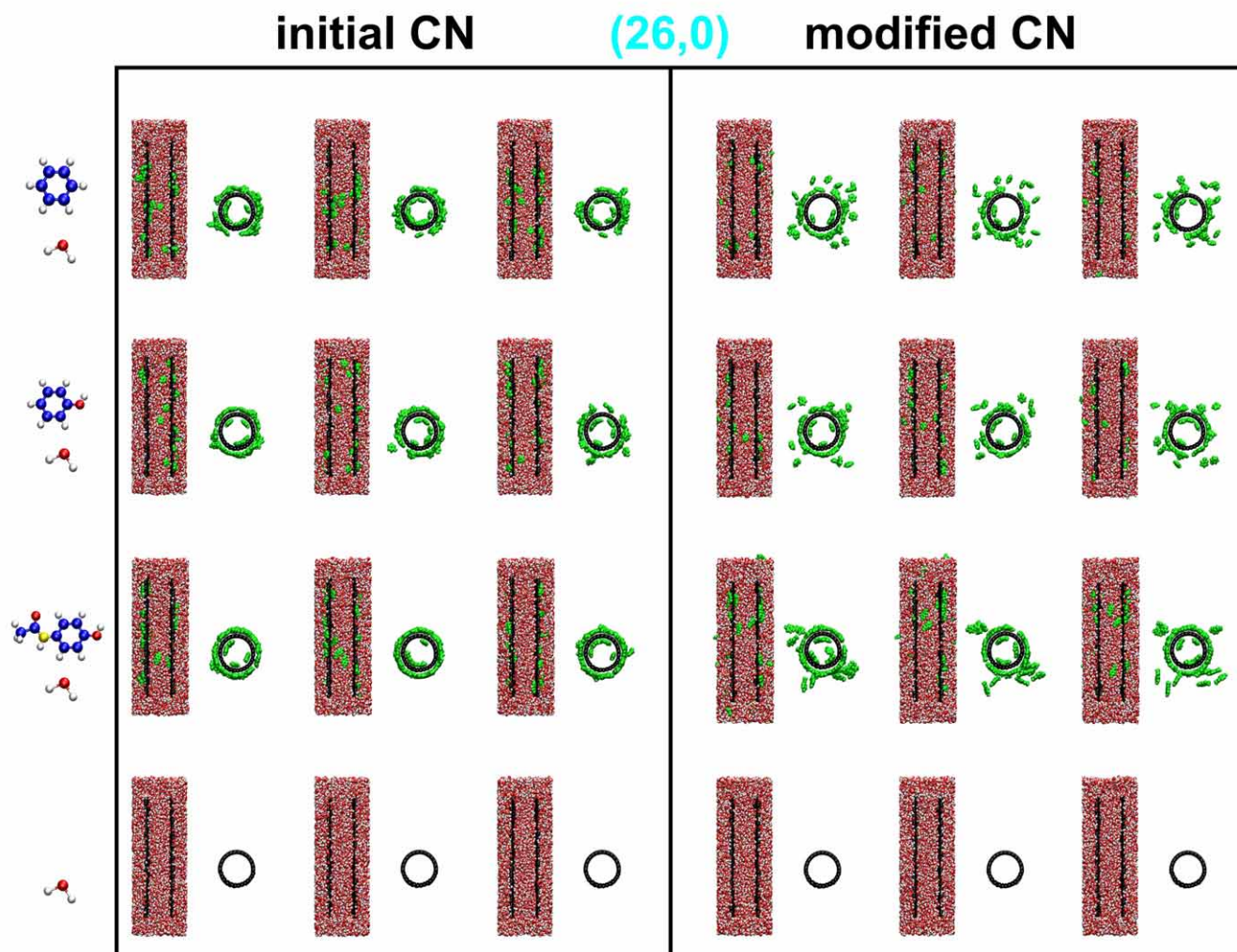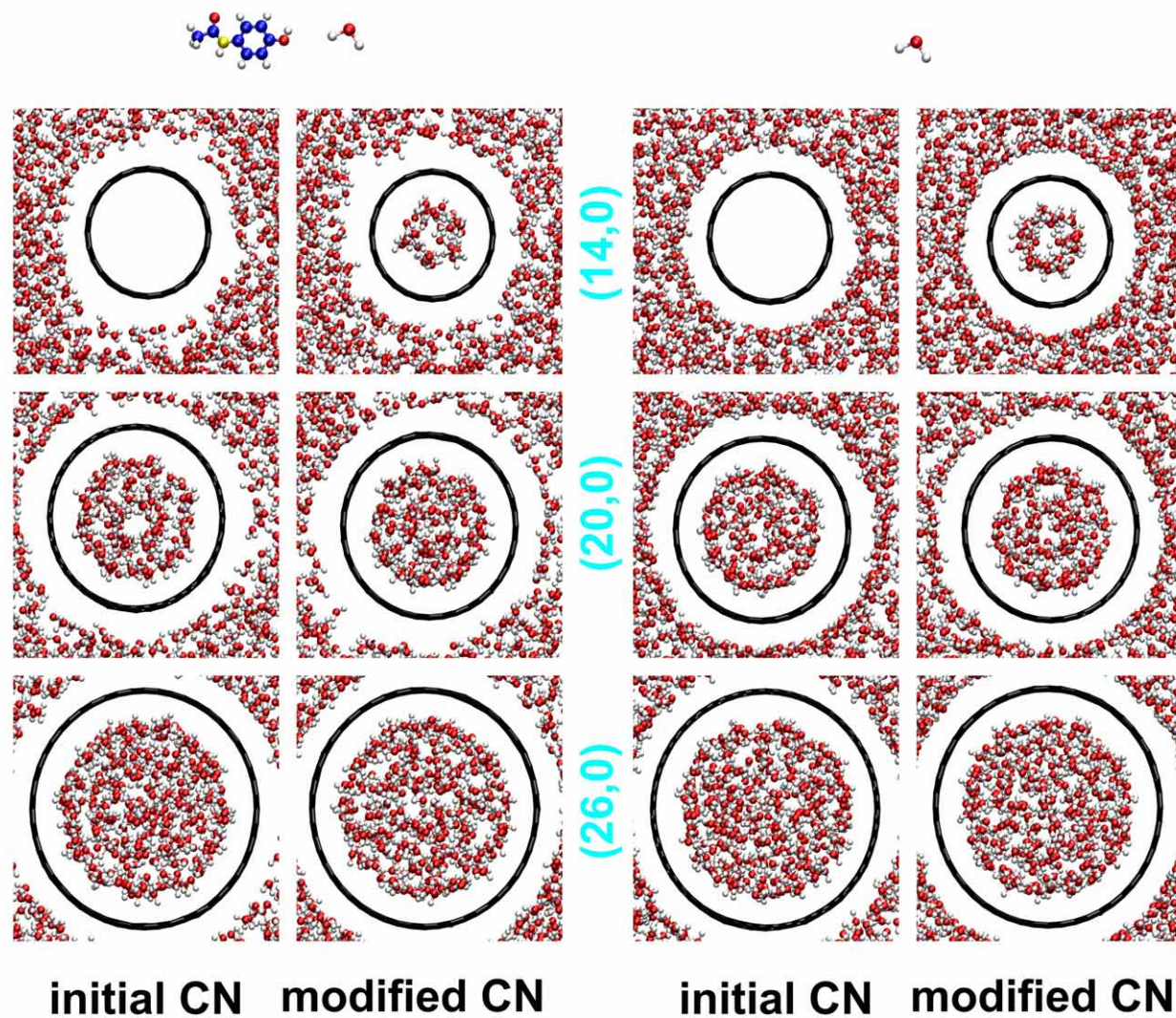
Figure S2. Equilibrium configurations for studied adsorbates, water and tubes (14,0).

Figure S3. Equilibrium configurations for studied adsorbates, water and tubes (20,0).

Figure S4. Equilibrium configurations for studied adsorbates, water and tubes (26,0).

Figure S5. Comparison of behaviour of water in the paracetamol-SWNT (left–adsorbate molecules were deleted) and water–SWNT (right) systems.