**Table ST1.** The optimized geometries (Å) of the pristine SWCNT as well as the functionalized carbon nanotube in the water solution.

|  |  |  |
| --- | --- | --- |
| Label | *f*-SWCNT | SWCNT |
| C34-C36 | 1.507 | 1.433 |
| C36-C25 | 1.505 | 1.421 |
| C35-C36 | 1.606 | 1.422 |
| C37-C35 | 1.505 | 1.433 |
| C46-C35 | 1.500 | 1.421 |

**Table ST2.** The optimized geometries (Å) of Gemcitabine molecule and the drug adsorbed at the functionalized complexes in the water solvent.

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | N113-H133 | N113-H132 | N112-C122 | N112=C122 | N112-C120 | C120=O110 | C117-O107 | C116-O107 | C115-F106 | O108-H128 | C118-O109 | O109-H130 |
| Gemcitabine | 1.008 | 1.006 | 1.341 | 1.326 | 1.357 | 1.229 | 1.405 | 1.436 | 1.352 | 0.965 | 1.410 | 0.966 |
| A | - | - | - | - | - | - | - | - | - | - | 1.409 | 0.981 |
| B | - | - | - | - | 1.355 | 1.233 | 1.407 | 1.437 | - | - | - | - |
| C | - | - | - | - | 1.356 | 1.233 | - | - | - | - | - | - |
| D | - | - | - | 1.325 | 1.358 | - | - | - | - | - | - | - |
| E | 1.009 | 1.007 | 1.342 | 1.327 | 1.358 | 1.230 | - | - | 1.366 | 0.986 | - | - |

**Table ST3.** The topological parameters (in a.u.) for Gemcitabine drug molecule and the adsorbed drug molecule in the studied complexes in the water solution.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Complex | Intramolecular Interaction | Complex |  | Gemcitabine |  |
|  |  |  **ρBCP** |  **∇2BCP** | **ρBCP** | **∇2BCP** |
| A | C118-O109 | 0.26315 | -0.44637 | 0.26498 | -0.41603 |
|  | O109-H130 | 0.34139 | -1.97183 | 0.36186 | -2.09810 |
|  | N112-C120 | 0.33647 | -1.18460 | 0.33087 | -1.14858 |
| B | C120=O110 | 0.39375 | 0.00711 | 0.40682 | 0.18248 |
|  | C117-O107 | 0.26790 | -0.50589 | 0.26731 | -0.51914 |
|  | C116-O107 | 0.24212 | -0.33288 | 0.24122 | -0.33506 |
| C | N112=C122 | 0.35329 | -1.17490 | 0.32610 | -0.93483 |
|  | N112-C120 | 0.33601 | -1.18037 | 0.36133 | -1.13375 |
| D | N112=C122 | 0.35446 | -1.17276 | 0.32610 | -0.93483 |
|  | N112-C120 | 0.33487 | -1.17727 | 0.36133 | -1.13375 |
|  | N113-H133 | 0.34037 | -1.83413 | \* | \* |
|  | N113-H122 | 0.33165 | -0.89560 | \* | \* |
|  | N112-C122 | 0.35343 | -1.18300 | 0.32610 | -0.93483 |
|  | N112-C120 | 0.33487 | -1.17471 | 0.33087 | -1.14858 |
| E | C120=O110 | 0.39625 | 0.02647 | 0.40682 | 0.18248 |
|  | C117-O107 | 0.27173 | -0.53576 | 0.26731 | -0.51914 |
|  | C116-O107 | 0.24385 | -0.31337 | 0.24122 | -0.33506 |
|  | C115-F106 | 0.25951 | 0.08079 | 0.26086 | 0.08534 |
|  | O108-H128 | 0.33350 | -1.95908 | 0.36087 | -2.11520 |