Supplementary data

**Table1:** The values of frequencies at wB97X-D/6-31G(d)

|  |  |
| --- | --- |
| Optimized structures | Frequency  (cm-1) |
| CNT (5.5) | + 64.74 |
| CNT(5.5) /Glyphosate | +10.58 |
| BNNT(5.5) | + 42.97 |
| BNNT(5.5)/Glyphosate | + 9.74 |

Table2: Adsorption energies (kJ/mol) for BNNT (5.5) / Glyphosate and BNNT (7.7) / Glyphosate.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Complexes | Adsorption energy (Eads) (kJ/mol) | | | |
| B3LYP/6-31G(d) | M06-2X/6-31G(d) | | ωB97X-D/6-31G(d) |
| BNNT(5.5)/Glyphosate | -31.68 | -57.99 | -67.21 | |
| BNNT (7.7)/Glyphosate | -29.01 | -55.99 | -66.47 | |

Table 3: Length effect on adsorption energies (kJ/mol) for BNNT (5.5) / Glyphosate.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Complexes | Adsorption energy (Eads) (kJ/mol) | | | |
| B3LYP/6-31G(d) | ωB97X-D/6-31G(d) | | M06-2X/6-31G(d) |
| B30H20N30 / Glyphosate | -31.68 | -67.21 | -57.99 | |
| B60H20N60 / Glyphosate | -29.62 | -82.92 | -72.63 | |



**Fig.1 :** The total electronic density of states (TDOS) obtained with the ωB97XD/6-31G (d) method.