**Table 1:** The Stoichiometry, electronic energy, enthalpy, Gibbs free energy (in Hartree), and dipole moment (Debye) of donepezil and its designed analogs.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound Name** | **Stoichiometry** | **Electronic Energy** | **Enthalpy** | **Gibbs free Energy** | **Dipole moment (Debye)** |
| Acyclovir | C9H13N4O3(2) | -795.14 | -795.14 | -795.20 | 7.561 |
| A |  |  |  |  |  |
| B |  |  |  |  |  |
| C |  |  |  |  |  |

**Table 2 (1)**: Energy of HOMOs, LUMO, gap, Hardness, and Softness (all units are in Hartree) For the Acyclovir **Beta MOs** and its designed analogs.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound Name** | **HOMO** | **LUMO** | **Gap** | **Hardness (n)** | **Softness** |
| Acyclovir | -0.19339 | -0.01701 | 0.17638 | 0.08819 | 11.34 |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

**Table 2(2)**: Energy of HOMOs, LUMO, gap, Hardness, and Softness (all units are in Hartree) For the Acyclovir **Alpha Mos** and its designed analogs.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound Name** | **HOMO** | **LUMO** | **Gap** | **Hardness (n)** | **Softness** |
| Acyclovir | -0.11793 | 0.00615 | 0.11178 | 0.05589 | 17.89 |
|  |  |  |  |  |  |
|  |  |  |  |  |  |