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**Supplementary Table 4: Energy calculation of different base pairing**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound | Energy (au) | Interaction E (au) | ∆G | kJ/mol |
| Adenine | -467.367 | NA | NA | NA |
| Cytosine | -394.988 | NA | NA | NA |
| Guanine | -542.633 | NA | NA | NA |
| Thymine | -454.204 | NA | NA | NA |
| AT | -921.591 | -0.020 | -12.240 | -39.000 |
| CG | -937.661 | -0.039 | -24.740 | -78.840 |
| AC | -862.354 | 0.001 | 0.740 | 2.370 |
| AC\_Reverse | -862.365 | -0.010 | -5.970 | -19.000 |
| AG | -1010.023 | -0.022 | -14.010 | -44.620 |
| CT | -849.208 | -0.016 | -10.340 | -32.950 |
| CT\_reverse | -849.214 | -0.022 | -13.500 | -43.020 |
| GT | -996.849 | -0.012 | -7.690 | -24.510 |
| GT\_reverse | -996.858 | -0.021 | -13.120 | -41.810 |