

Supplementary Material

Density Functional Computations on 6-Aminouracil: Effect of Amino Group in the 6th Position on the Watson–Crick Base Pair Uridine–Adenosine

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Table 1-Sup. Energy values in a.u. obtained in the complexes with dA of Figs. 5–7.

| | total | Ur, 5-aminoUr, 6-aminoUr optimized | Ur, 5-aminoUr, 6-aminoUr frozen | dA optimized | dA frozen |
|--------------------|--------------|------------------------------------|---------------------------------|--------------|-------------|
| Fig 5 6-aminoUr:dA | -1854.766527 | -966.399256 | -966.397476 | -888.340189 | -888.339174 |
| Fig 6 Ur:dA | -1799.413193 | -911.046649 | -911.044894 | -888.340189 | -888.339284 |
| 5-aminoUr:dA | -1854.767948 | -966.401888 | -966.400177 | -888.340189 | -888.339336 |
| 6-aminoUr:dA | -1854.777794 | -966.411109 | -966.409395 | -888.340189 | -888.339233 |
| Fig. 7 Ur:dA | -1799.415620 | -911.048137 | -911.046090 | -888.340189 | -888.339312 |
| 5-aminoUr:dA | -1854.771211 | -966.404302 | -966.402307 | -888.340189 | -888.339356 |
| 6-aminoUr:dA | -1854.777584 | -966.409692 | -966.407693 | -888.340189 | -888.339206 |