

Covalent Organic Framework (C₆N₆) as a Drug Delivery Platform for Fluorouracil to Treat Cancerous Cells: A DFT Study

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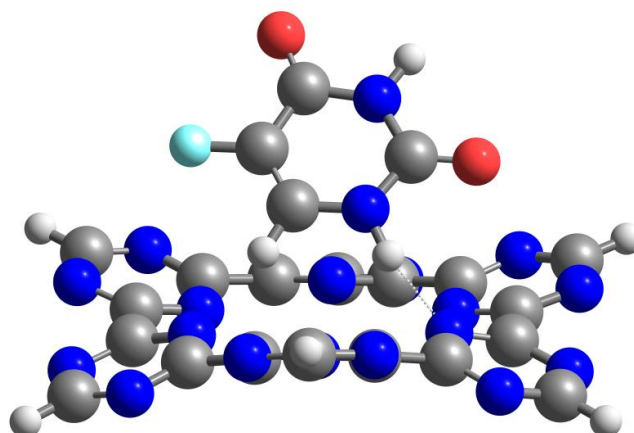
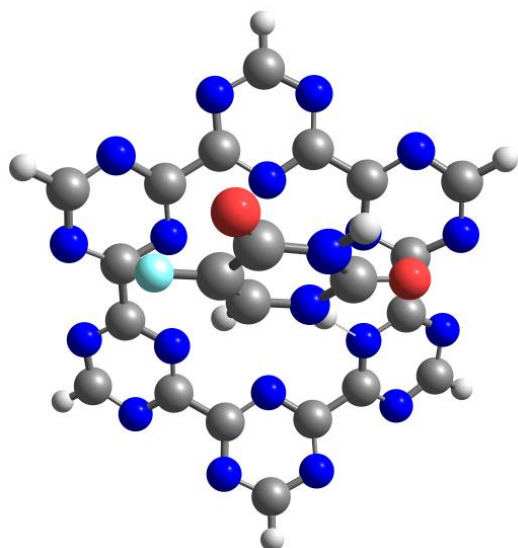
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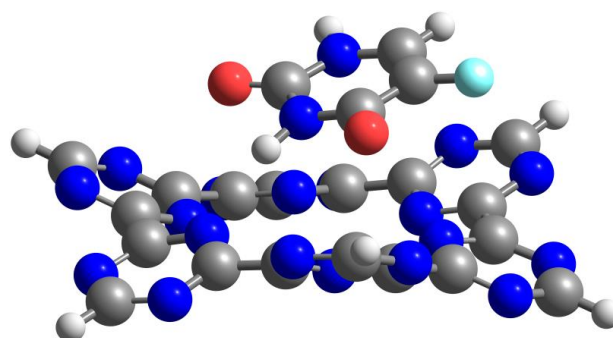
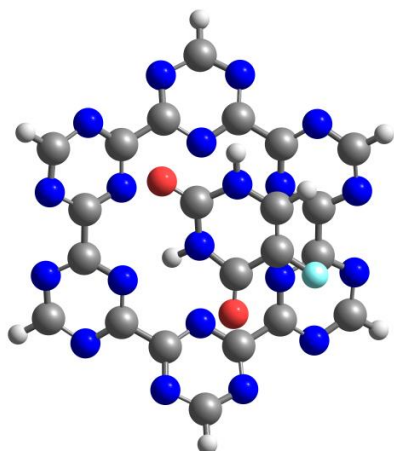
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Table S1. Adsorption energies of least stable complexes of drug@C₆N₆.

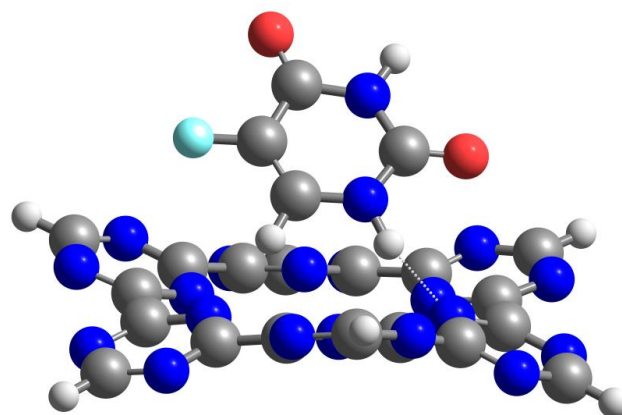
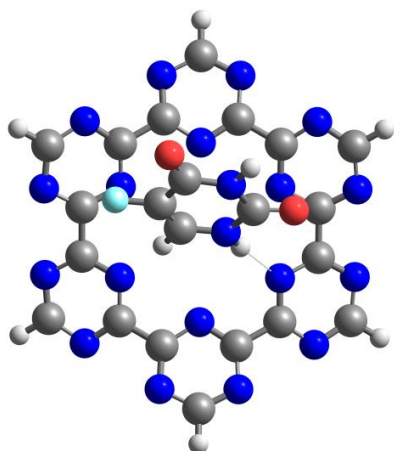
| Drug@C ₆ N ₆ | Adsorption energies |
|------------------------------------|---------------------|
| A | -28.13 |
| B | -23.02 |
| C | -28.10 |
| D | -26.55 |
| E | -19.35 |
| F | -19.35 |



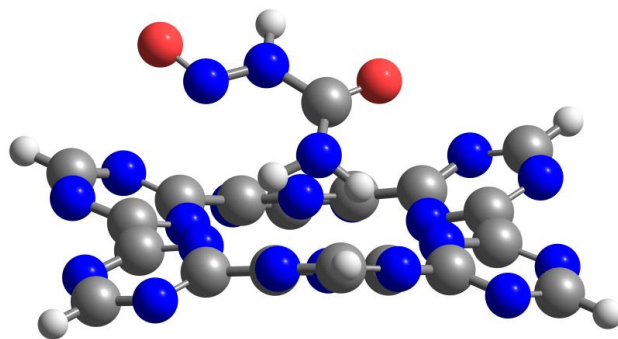
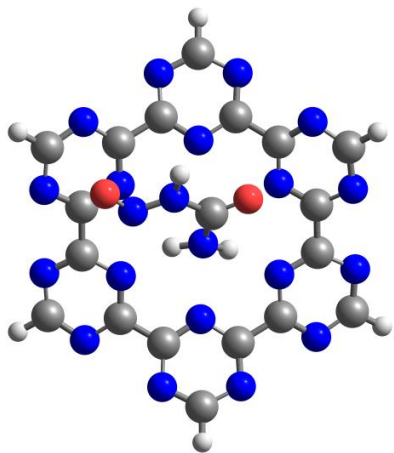
A



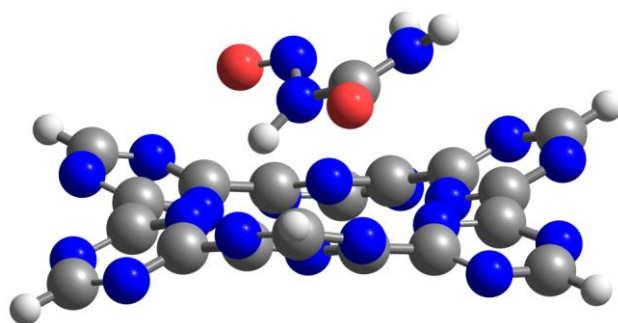
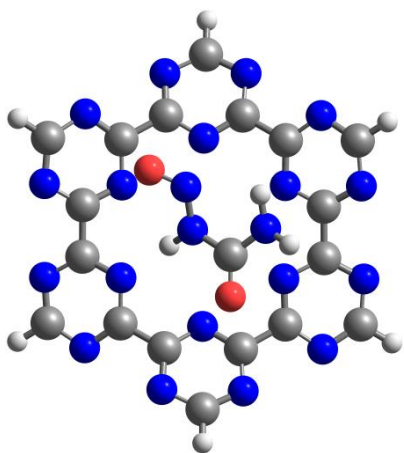
B



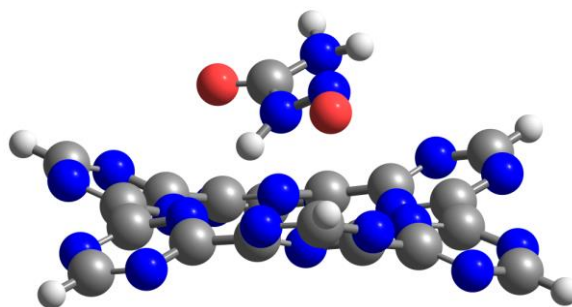
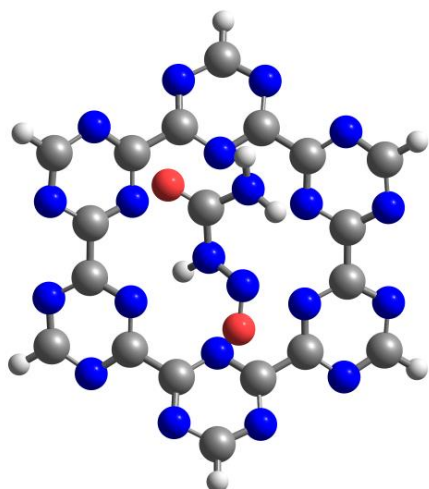
C



D



E



F

Figure S1. Top and side views of least stable complexes of FU@C₆N₆ (A–C) and NU@C₆N₆ (D–F).