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Supporting information

Two-dimensional covalent triazine frameworks as a superior nanocarrier for drug delivery of thioguanine anti-cancer drugs: A periodic DFT study

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Table S1.

Corresponding bond lengths for the optimized S1-S9 complexes.	
Complexes	Bond length
S1	Average distance between the TG drug and the CTF sheet: 2.8-3.4 Å
S2	Average distance between the TG drug and the CTF sheet: 3.1-3.4 Å
S3	S_{drug}---H_{CTF} = 3.1 Å
S4	S_{drug}---H_{CTF} = 3.2 Å
S5	S_{drug}---H_{CTF} = 2.7 Å
S6	Distance between the hydrogen atom attached to the nitrogen No. 4 of the drug and the carbon atom of the R3 ring of the CTF sheet: 2.4 Å
S7	-NH_{2drug}---N_{CTF} = 2.6 Å
S8	-NH_{2drug}---C_{CTF} = 2.7-2.9 Å
S9	S_{drug}---N_{CTF} = 3.3 Å

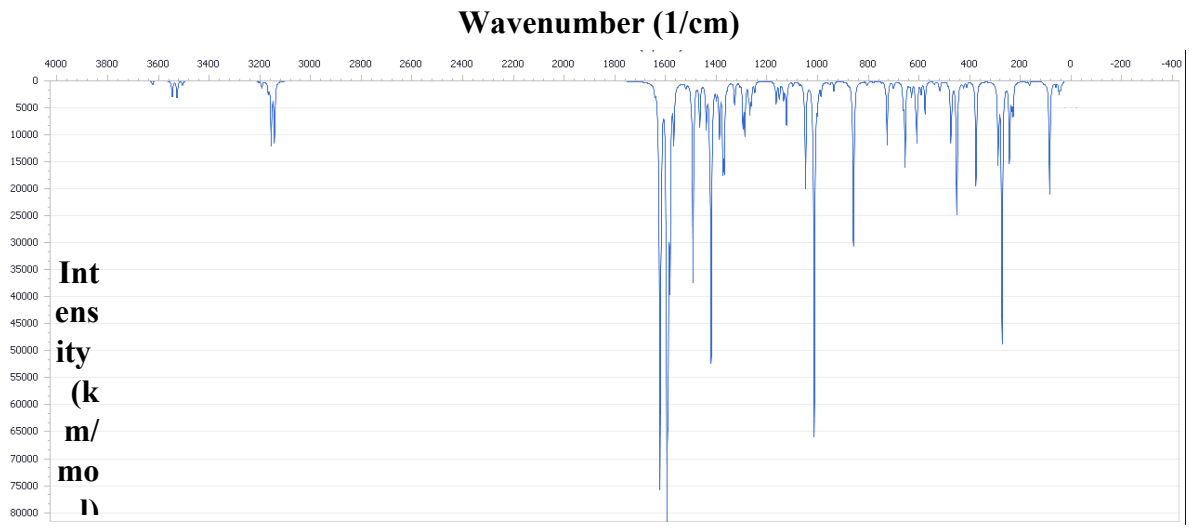

Figure S1. IR spectrum of the most stable S1 complexes.