

## **Supplementary information: Elucidating Anticancer Drug Release from UiO-66 as a Carrier through the Computational Approaches**

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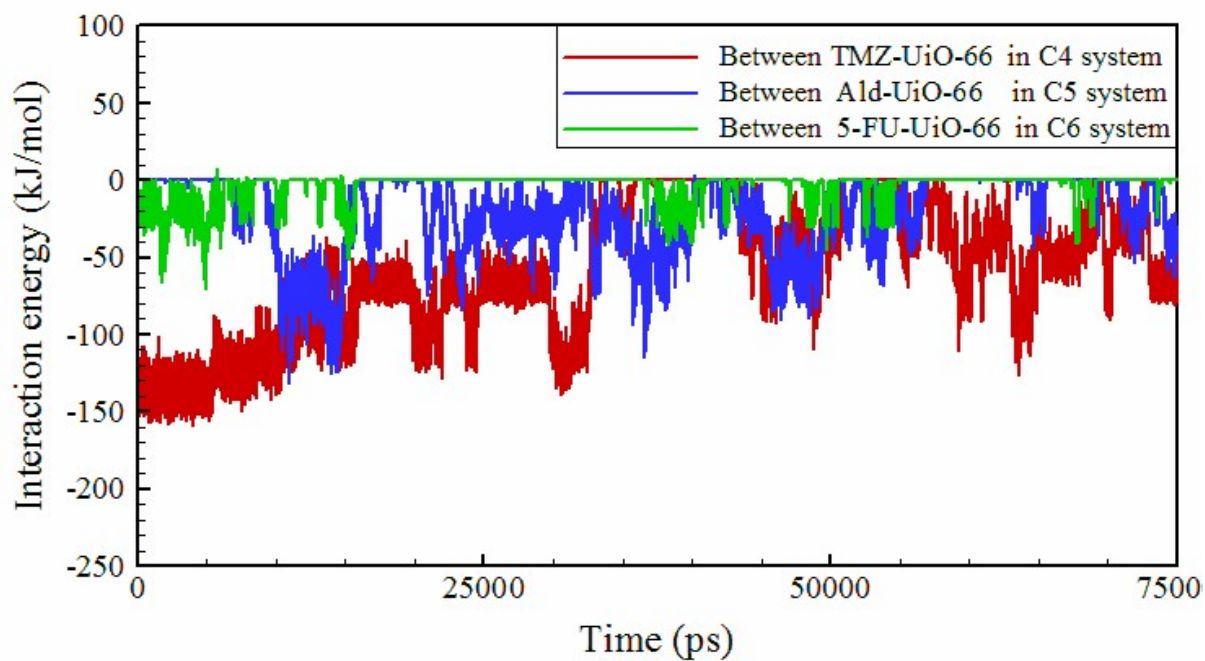
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## 1. Interaction energies



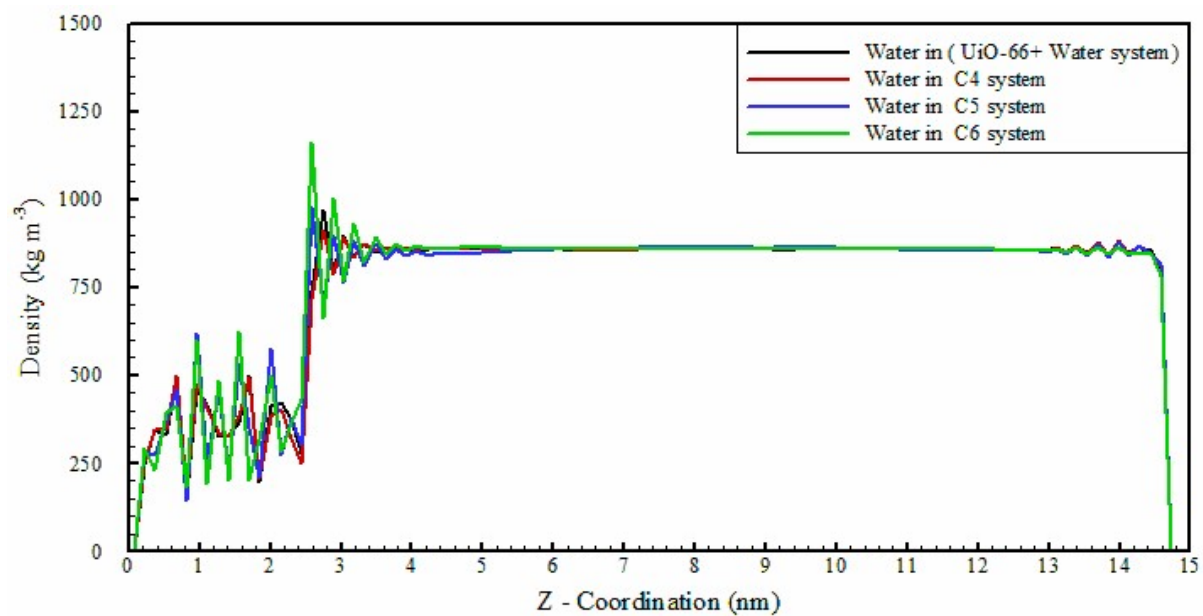
**Figure S1.** The interaction energy between drug and UiO-66 in simulated systems

**The system C4 consists of TMZ + UiO-66 + Water**

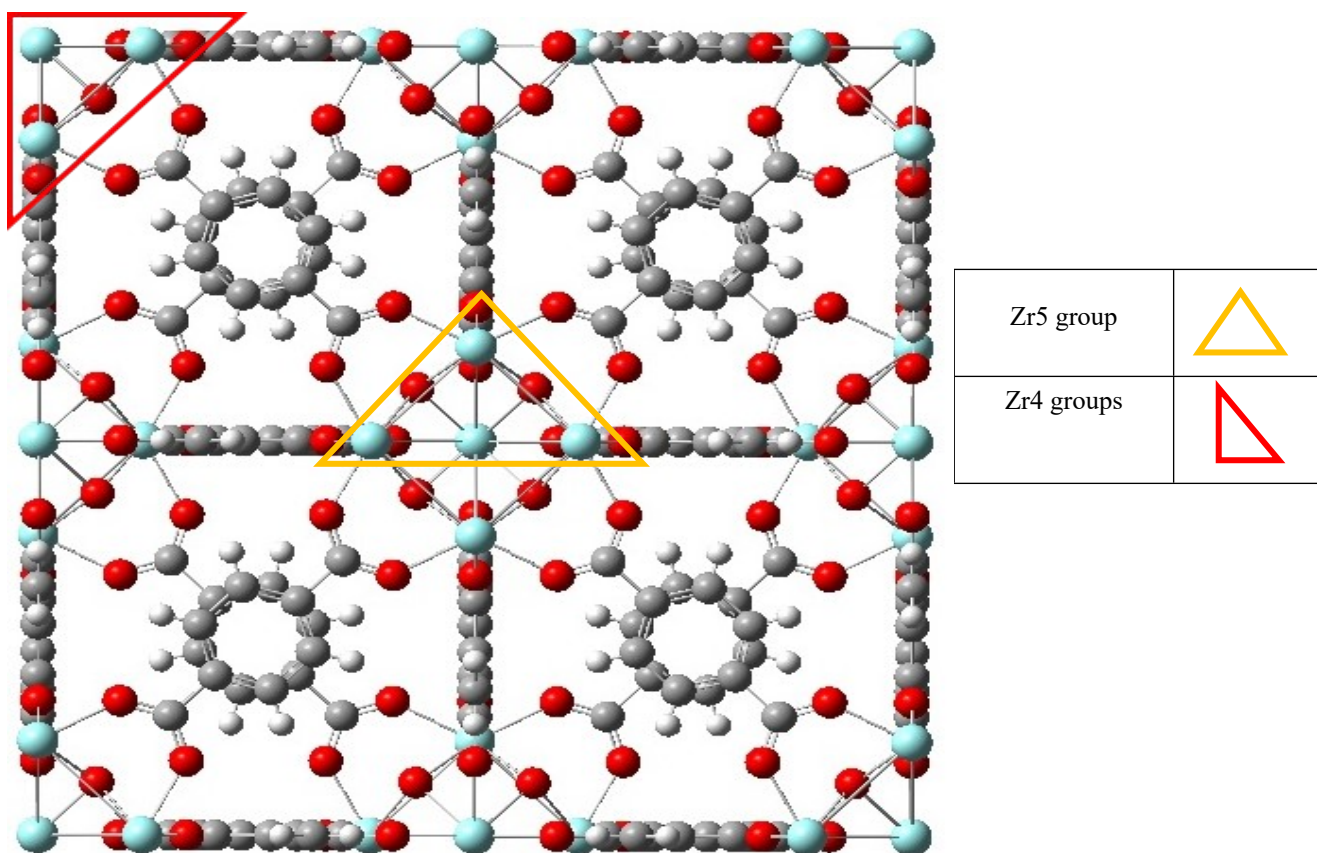
**The system C5 consists of Ald + UiO-66 + Water**

**The system C6 consists of 5-FU + UiO-66 + Water**

## 2. Density profile in UiO-66



**Figure S2.** The profile of density of water in different simulated systems.



**Figure S3:** Visualization of Zr atom positions in UiO-66 structure.

**Table S1.** Number of contacts in different simulated systems in 300 K and 313 K.

	<b>Property Systems</b>	<b>Number of Contact between Zr5 and water molecules</b>	<b>Number of Contact between Zr6 and water molecules</b>
<b>T=300 K</b>	<b>TMZ/water/UiO-66</b>	1.222( $\pm$ 0.005)	1.179( $\pm$ 0.033)
	<b>Ald/water/UiO-66</b>	1.404( $\pm$ 0.006)	1.406( $\pm$ 0.008)
	<b>5-Fu/water/UiO-66</b>	0.992( $\pm$ 0.004)	0.977( $\pm$ 0.005)
<b>T=313 K</b>	<b>TMZ/water/UiO-66</b>	1.179( $\pm$ 0.898)	1.128( $\pm$ 0.888)
	<b>Ald/water/UiO-66</b>	1.208( $\pm$ 0.917)	0.278( $\pm$ 0.235)
	<b>5-Fu/water/UiO-66</b>	0.910( $\pm$ 0.773)	0.955( $\pm$ 841)