Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Electronic Supplementary Information

for

Computational Investigation of Metal Organic Frameworks for Storage and Delivery of Anticancer Drugs

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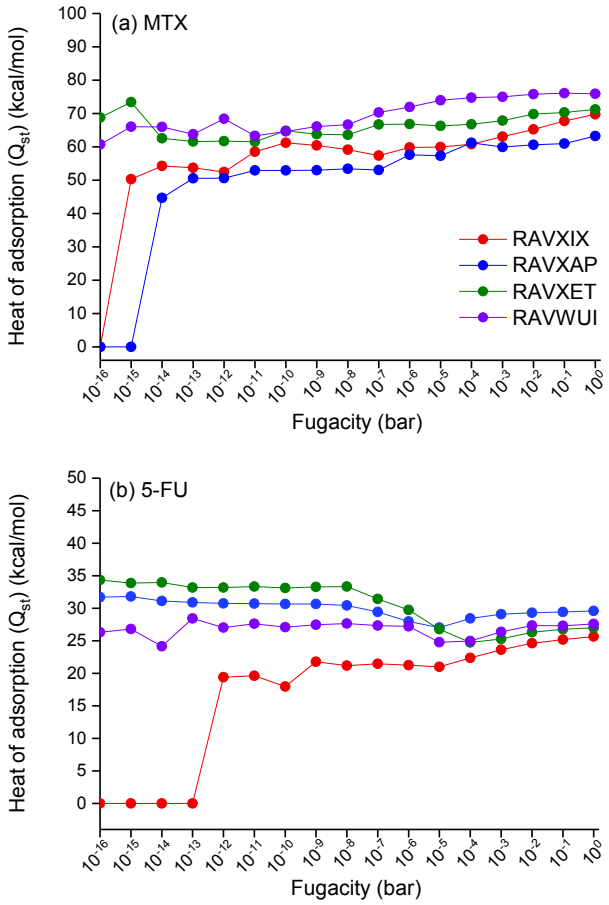

Figure S1. The heat of adsorption as a function of fugacity for (a)MTX and (b)5-FU adsorption in MOFs, RAVXIX, RAVXAP, RAVXET and RAVWUI.

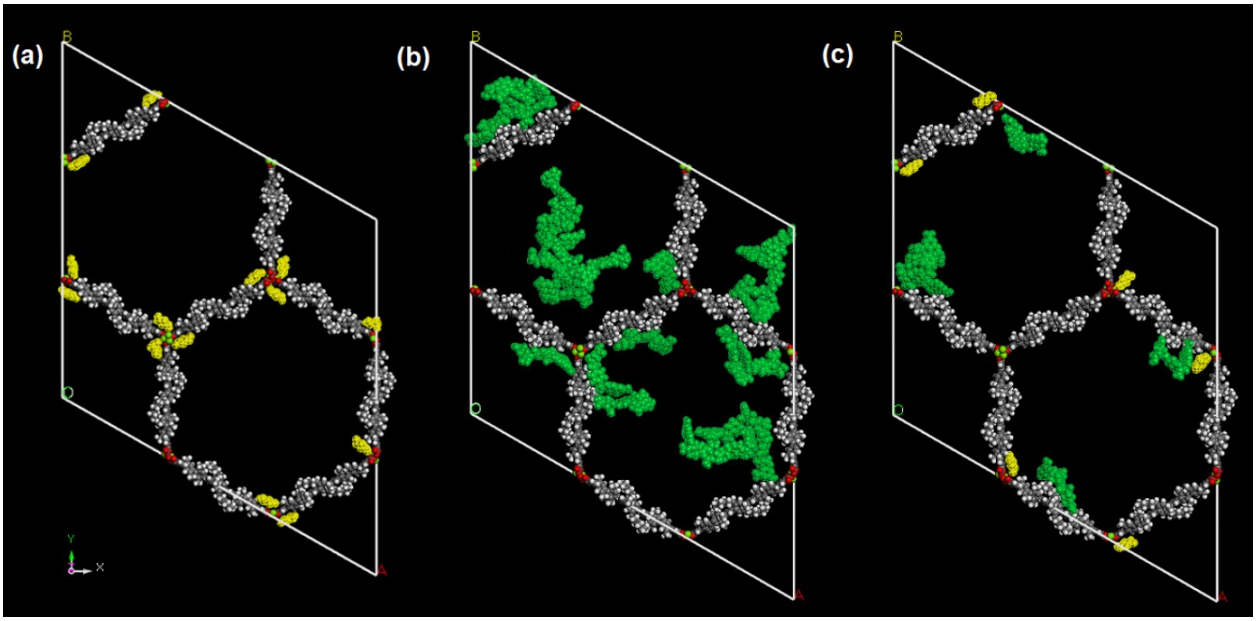

Figure S2. Snapshots of drug adsorption simulations in RAVXIX: (a)5-FU, (b)MTX and (c)5-FU/MTX mixture. 5-FU (MTX) molecules are shown with yellow (green) space-filling model.

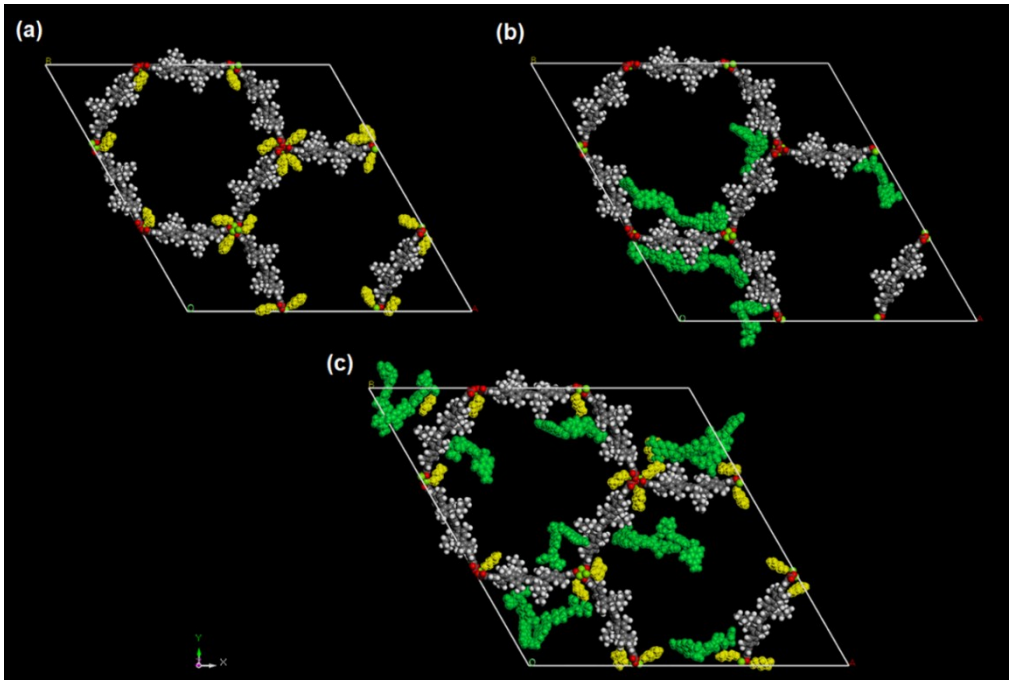

Figure S3. Snapshots of drug adsorption simulations in RAVXAP: (a) 5-FU, (b) MTX and (c) 5-FU/MTX mixture. 5-FU (MTX) molecules are shown with yellow (green) space-filling model.

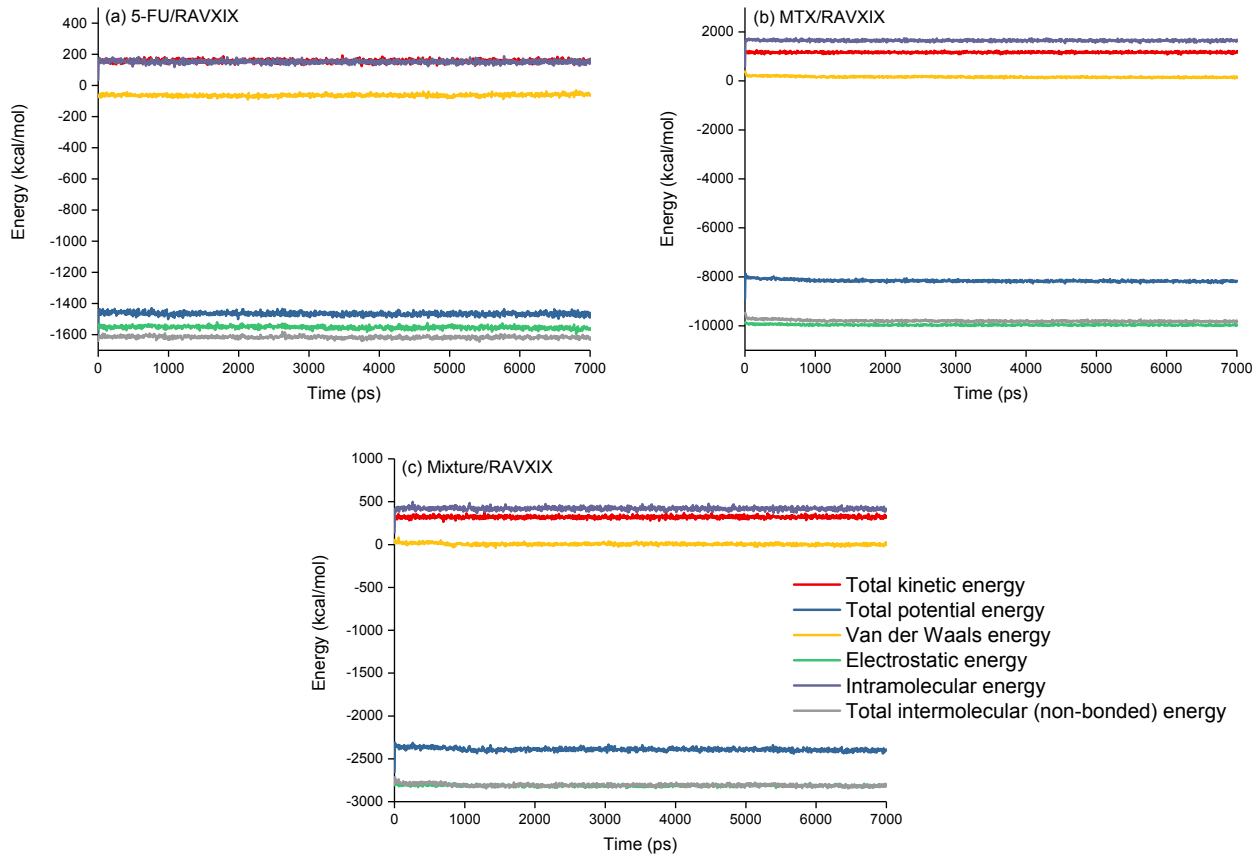

Figure S4. Energy analysis of RAVXIX during MD simulations.

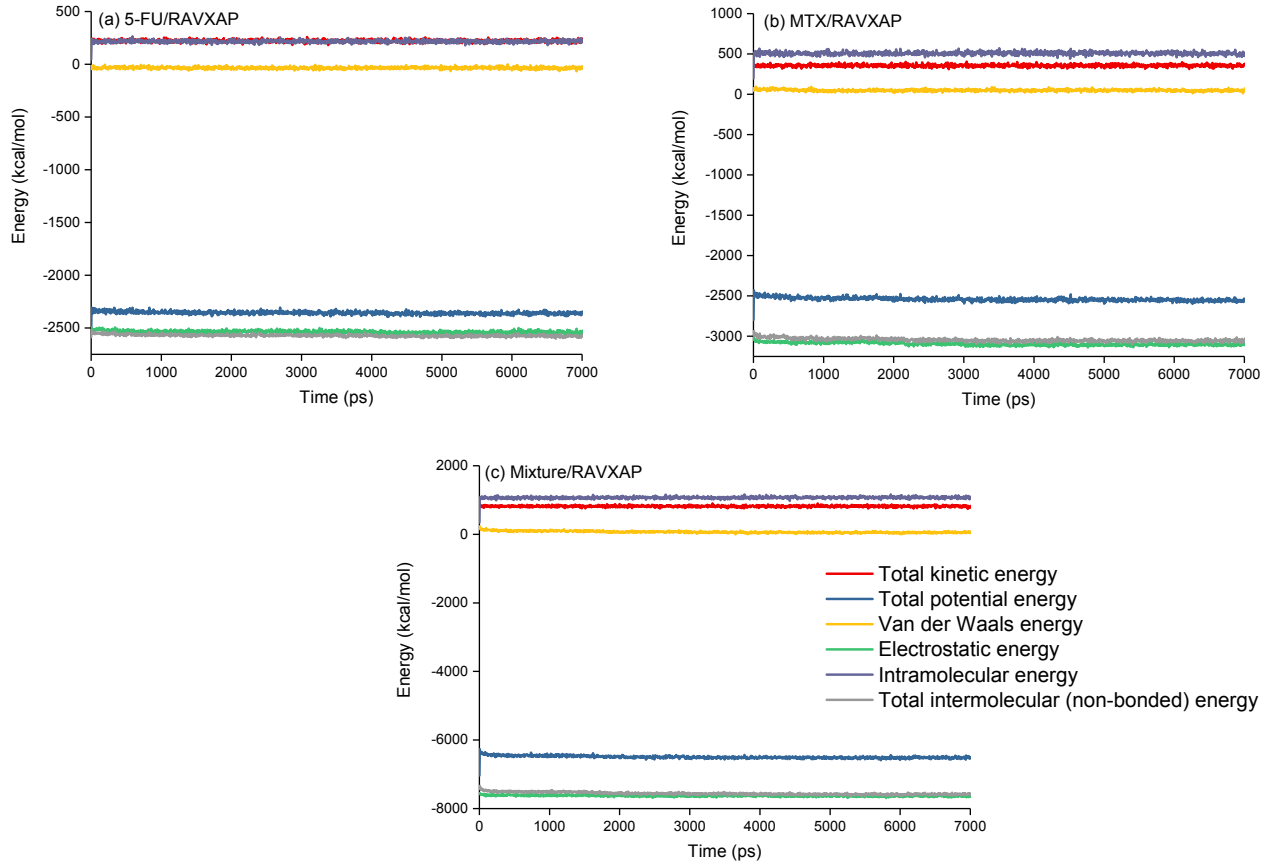

Figure S5. Energy analysis of RAVXAP during MD simulations.