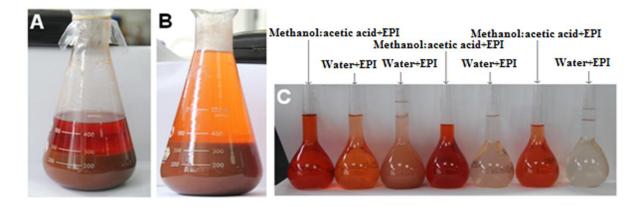
## **Supporting information**

Anticancer loading and controlled release on novel water-compatible magnetic nanomaterials as drug delivery agent, coupled to computational modeling approach

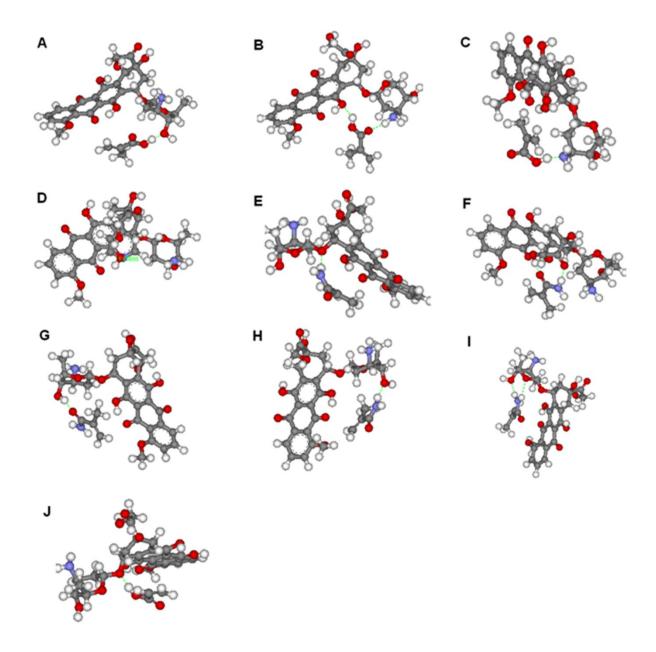
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**Fig. S1** Photograph of the washing process just after finish to prepare the M-MIPs: (A) First supernatant solvent separated with the nanomaterials by precipitation couplet with the magnet; (B) Color of the separation stat after washing several times with water; (C) In order from left to right, samples of the washing supernatant interchanging methanol-acetic acid and water.



**Fig. S2** Additional chemical structures of interaction mode of Complex monomer-EPI: (A) EPI-MAA1, (B) EPI-MAA2, (C) EPI-MAA3, (D) EPI-4VP, (E) EPI-AA1, (F) EPI-AA2, (G) EPI-AA3, (H) EPI-AA4, (I) EPI-AA5, (J) EPI-MAM. Hydrogen bonds are represented by green dotted lines.