

Electronic Supplementary Information for:

Multiple noncovalent interactions mediated one-pot therapeutic assemblies for effective treatment of atherosclerosis

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Table S1. Estimated binding energy values using different searching algorithms.

Algorithm	Estimated binding energies (kcal/mol)	
	RAP	IND
GA	-4.63	-3.18
LGA	-5.8	-5.0
LS	-4.38	-2.79
SA	-2.26	-2.11

It should be noted that LGA predicted the strongest affinity between PNIPAm and IND or RAP.

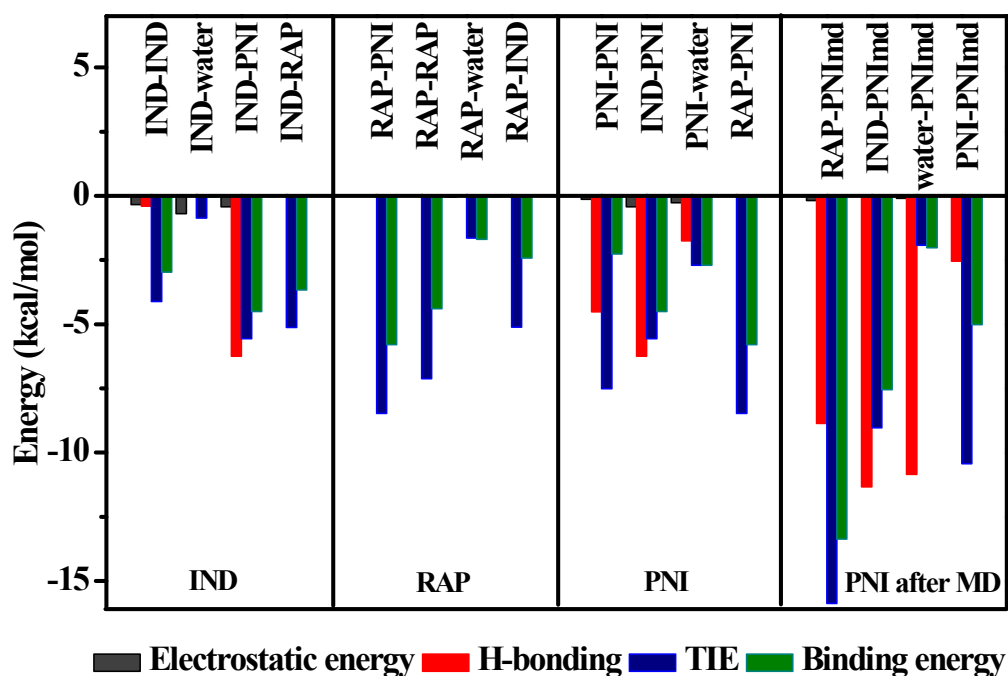


Figure S1. Calculated values of intermolecular energies and binding energy between two component pairs of IND, RAP, initially minimized conformation of PNIPAm (PNI), conformation of PNIPAm after a MD stimulation (PNI_{md}) and water. TIE represents the total intermolecular energy including van der Waals forces, H-bonding, and desolvation interaction.

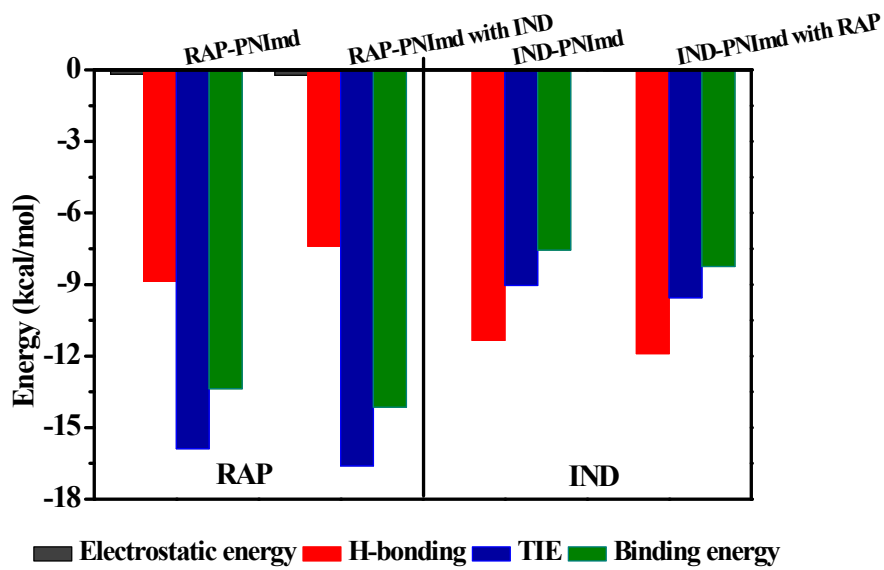


Figure S2. Estimated values of intermolecular energies and binding energy between RAP and PNIPAm with or without IND as well as those between IND and PNIPAm with or without RAP. TIE means the total intermolecular energy including van der Waals forces, H-bonding, and desolvation interaction.

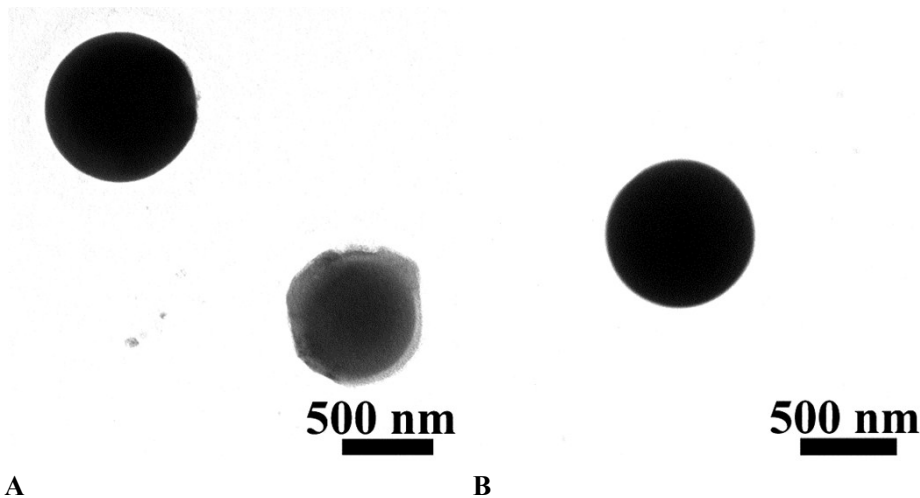


Figure S3. TEM images of RAP microspheres fabricated by an emulsion technique using PLGA (A) or S100 (B). The mean size of RAP/PLGA and RAP/S100 microspheres was 672 ± 11 and 668 ± 44 nm, while the RAP loading content was 18.1% and 17.2%, respectively.

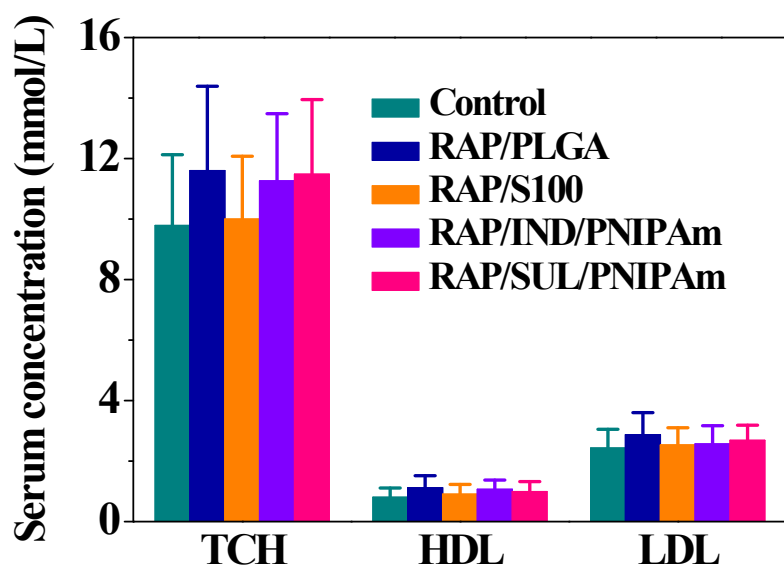


Figure S4. The serum levels of typical lipids. TCH, total cholesterol; LDL, low-density lipoprotein; and HDL, high-density lipoprotein. Data are mean \pm S.D. (n = 6).