Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary information

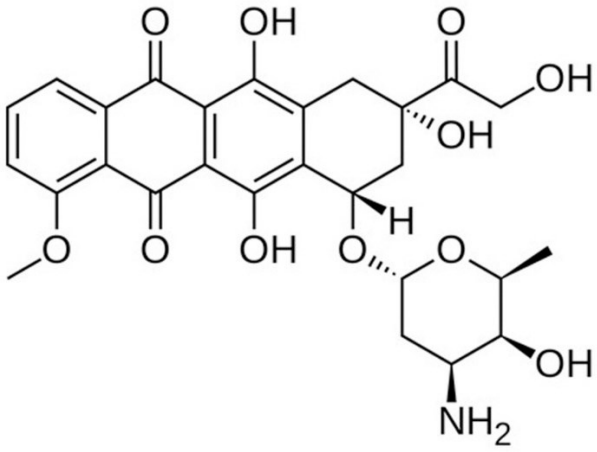
Molecular Engineering of the Last-Generation CNTs in Smart Cancer therapy by Grafting PEG–PLGA- Riboflavin

Somayeh Sohrabi[a], Mohammad Khedri[a], Reza Maleki[b], Mostafa Moraveji[a,*]

[a] Department of Chemical Engineering, Amirkabir University of Technology (Tehran Polytechnic), 424 Hafez Avenue, Tehran, 1591634311, Iran

[b] Computational Biology And Chemistry Group (CBCG), Universal Scientific Education and Research Network (USERN), Tehran, Iran

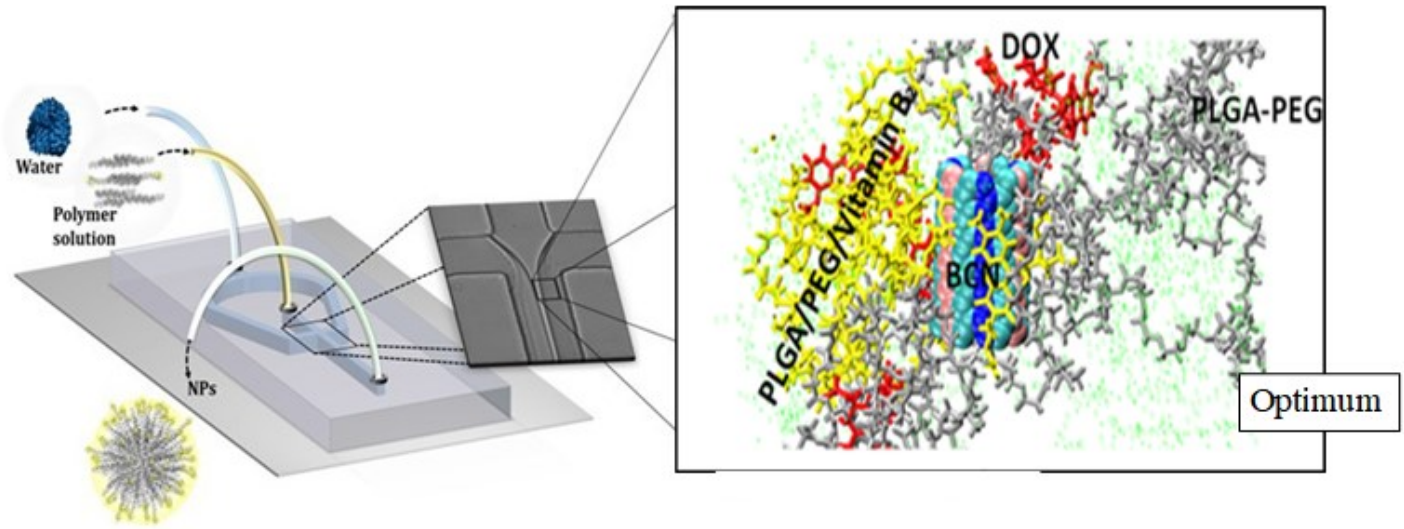
*Corresponding author's email: moraveji@aut.ac.ir



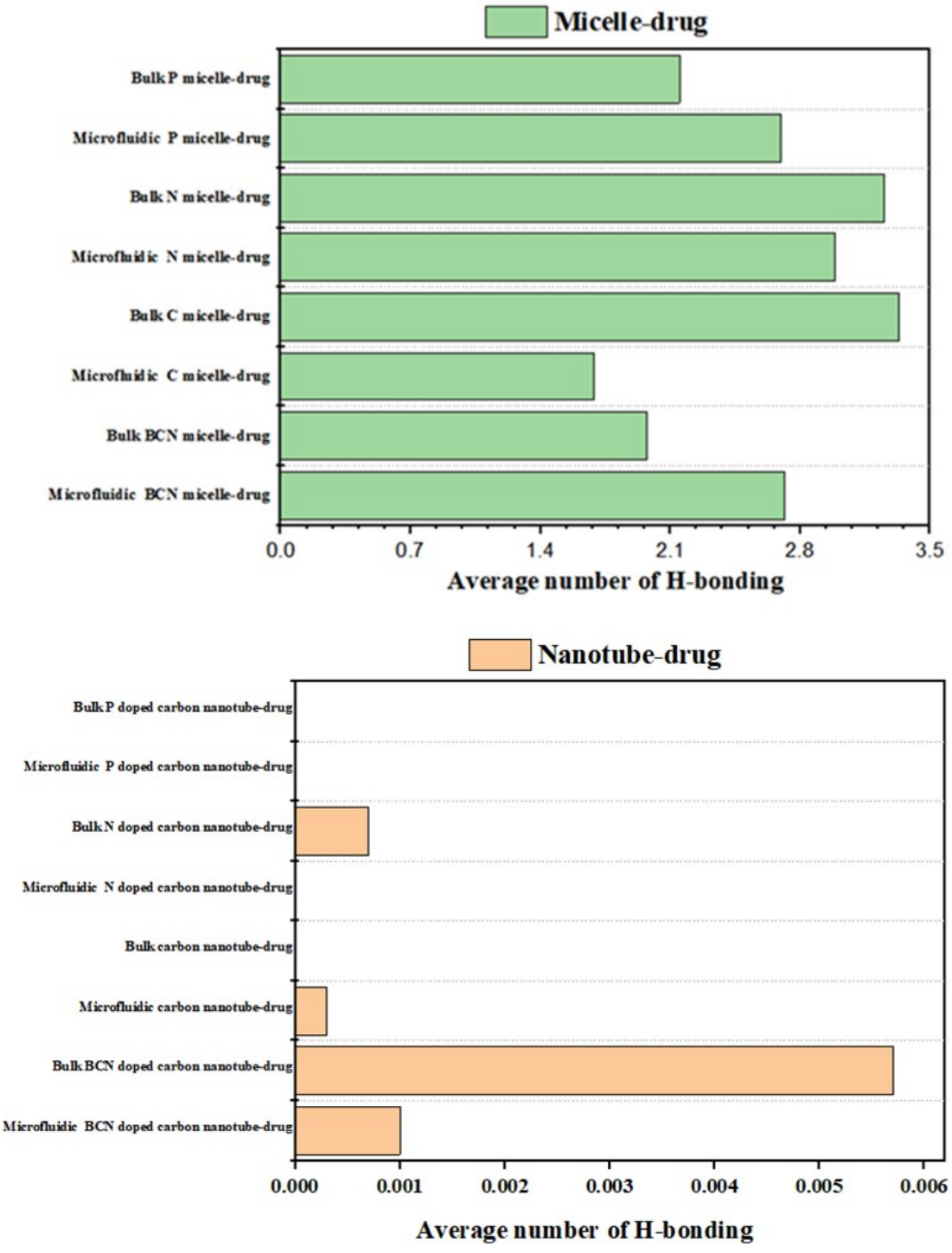
Supplementary Figure S1. Chemical structure of doxorubicin (Dox) anticancer drug [1].

Supplementary Table S1.

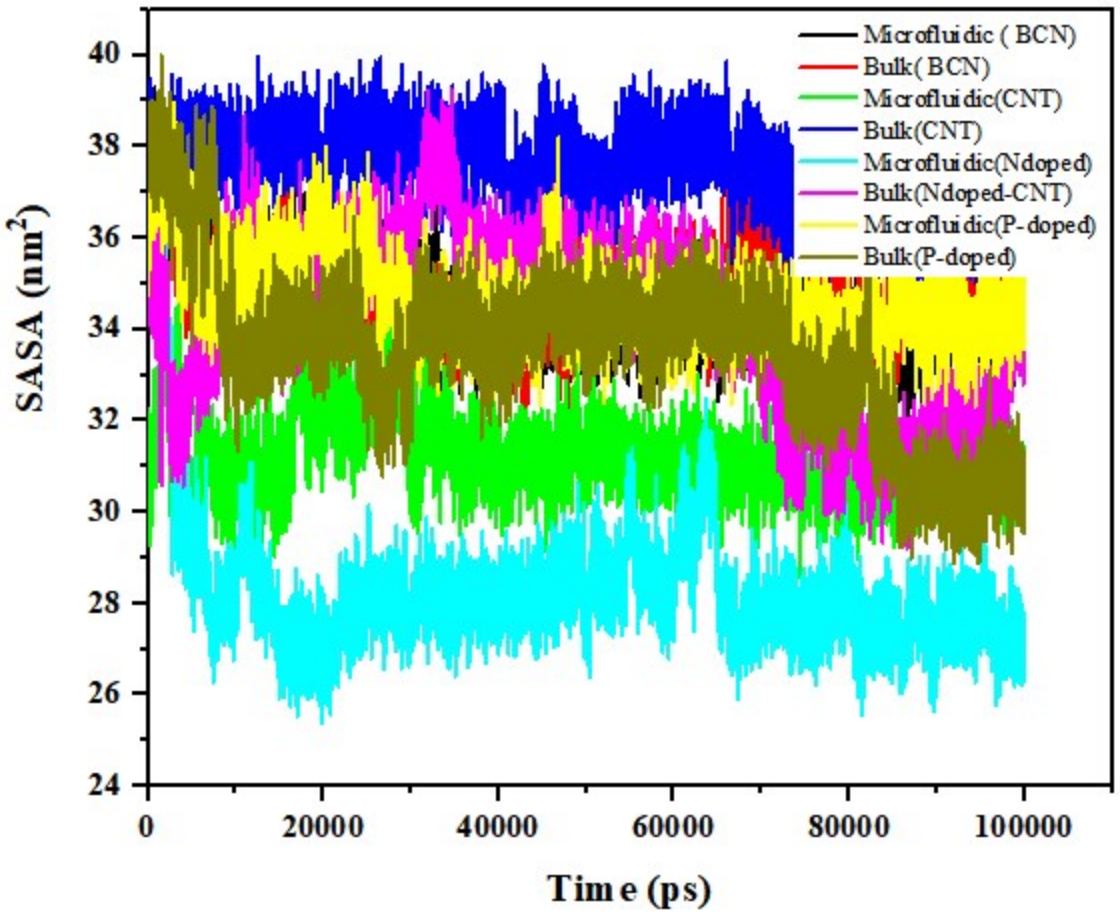
Dopant Concentration	Gibss Free Energy	
	N- doped-CNT	P- doped-CNT
5	-7.62	-9.04
8	-10.36	-12.14
10	-12.64	-13.46
15	-11.29	-11.91
20	-6.57	-7.89



Supplementary Figure S2. The flow-focusing microfluidics system for DOX delivery



Supplementary Figure S3. Average number of hydrogen bonds in PLGA/PEG/RF@ (doped)/DOX in bulk and microfluidic systems



Supplementary Figure S4. The SASA trends for DOX in the presence of doped CNT in bulk and microfluidic system