Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Nanoarchitectures by hierarchical self-assembly of ursolic acid: entrapment and release of fluorophores including anticancer drug doxorubicin

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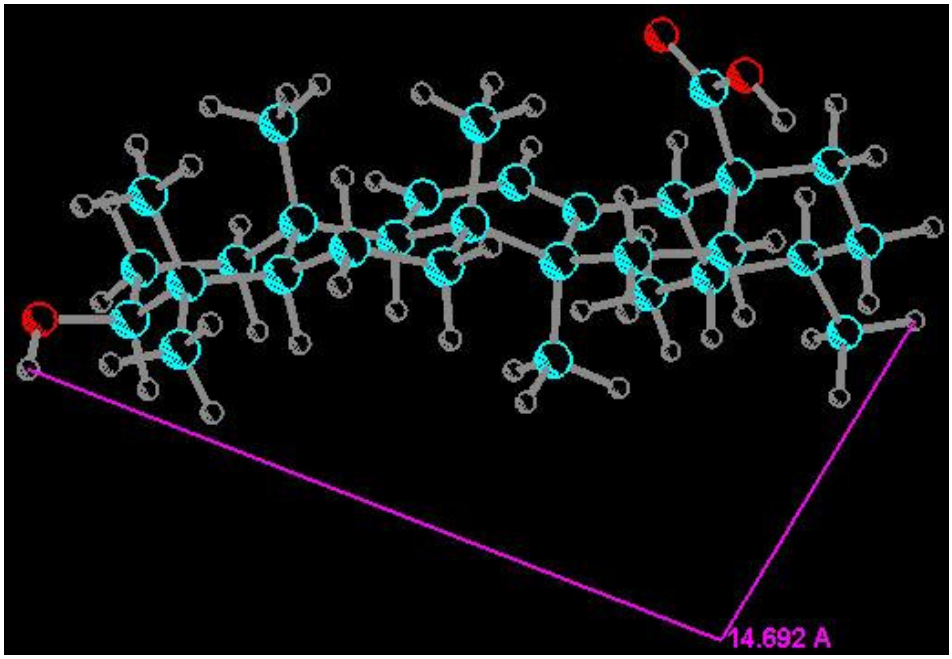

Fig. S1: Energy minimized structure of ursolic acid **1** using MMX force field as implemented in PC MODEL version 9.2 (Serena Software)

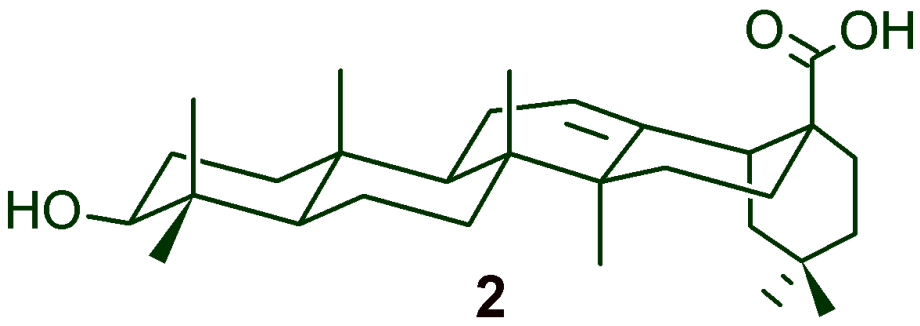

Fig. S2: structure of oleanolic acid

Table TS1: Gelation Test Results of **1** in organic solvents

Entry	Solvent	State	MGC	T_{gel} (°C)
1	o- Xylene	G	1.64	35.1
2	m-Xylene	G	1.04	33.2
3	Mesitylene	G	1.41	63.2
4	Toluene	CS	2.0	-
5	Bromo benzene	G	3.25	51.2
6	Chloro benzene	G	4.01	57
7	o-dichloro benzene	G	1.0	37.4
8	Nitro benzene	CS	1.02	-
9	CCl_4	I	<1	-
10	ETOH	CS	1.25	-
11	MeOH	CS	1.21	-
12	n-Propanol	CS	2.14	-
13	Isopropanol	C	2.0	-
14	n- butanol	G	5.21	42.2
15	n-pentanol	G	4.51	48.5
16	n-hexanol	G	6.25	50.1
17	n-heptanol	G	5.12	55.2
18	n-octanol	G	4.8	59.1
19	n-decanol	CS	2.12	-
20	Ethylene glycol	CS	1.33	-
21	DMF	S	10	-
22	DMSO	G	1.34	39.1

Gelation tests were carried out with a maximum concentration of 10% w/v. MGC is the minimum gelator concentration at which the gel formed at room temperature. G = gel,CS = colloidal suspension, C= crystal, S = solution.

Table TS2: Gelation Test Results of **1** in mixed solvents:

Entry	Solvent	MGC	State	T_{gel} (°C)
1	3:1 Ethanol/H_2O	1.27	CS	-
2	5:1 DMSO/H_2O	2.12	G	42.2
3	5:1 DMF/H_2O	3.55	CS	-

Gelation tests were carried out with a maximum concentration of 10% w/v. MGC is the minimum gelator concentration at which the gel formed at room temperature. G = gel, CS = colloidal suspension.

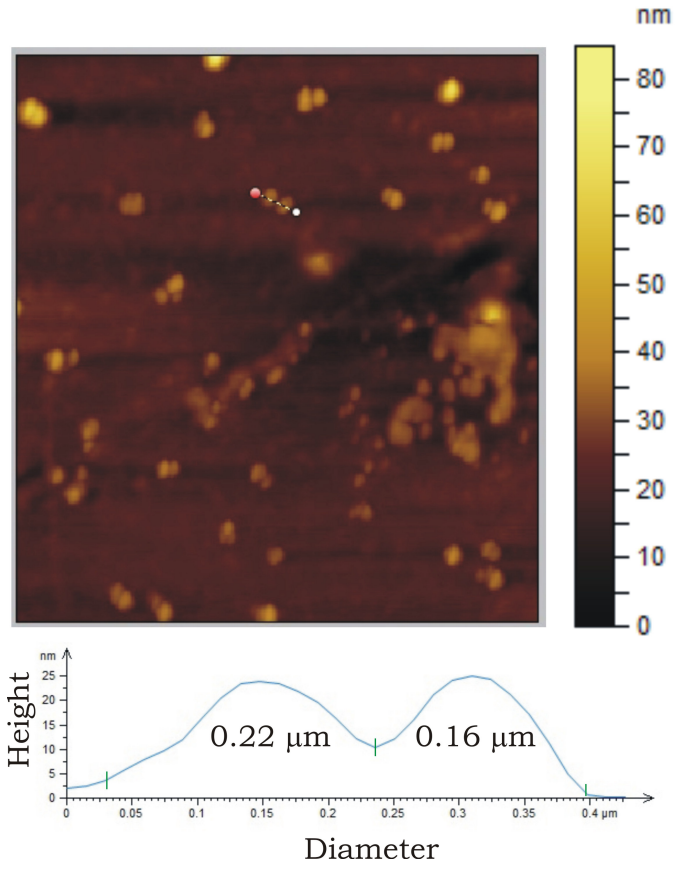

Fig. S3: AFM images (a: 2D, b: 3D) of the self-assemblies of ursolic acid in PhCl (0.10 % w/v), (c) height vs diameter plot.

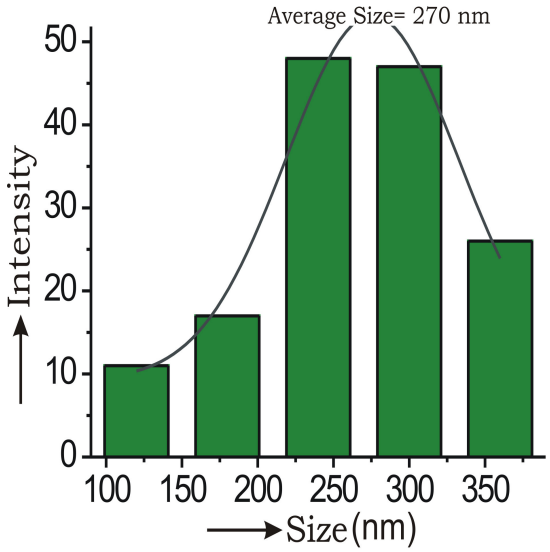

Fig. **S4:** Histogram of self-assemblies of **1** in ethanol-water (3:1. 0.11 % W/V) observed by AFM.

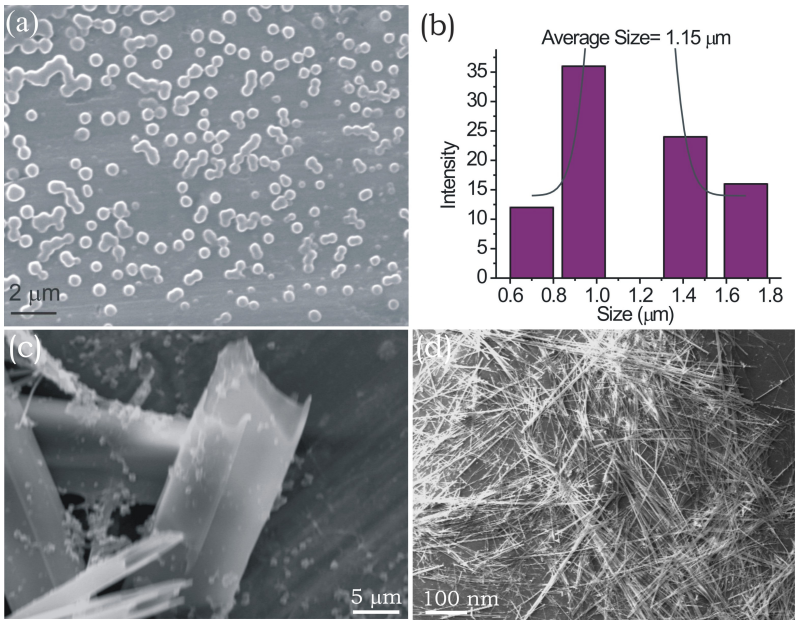

Fig. S5: Scanning electron micrographs of dried self-assemblies of ursolic acid in ethanol-water (3:1): (a) 0.115 % (w/v), (b) histogram of (a), (c, d) 0.23 % (w/v).

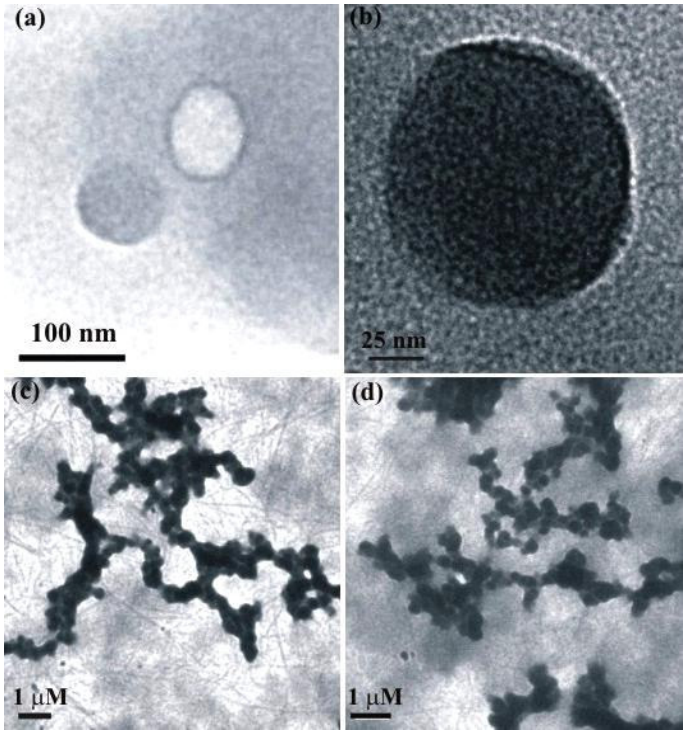

Fig. S6: HRTEM (unstained) images of self-assemblies of ursolic acid in (a,b) ethanol-water (3:1, 0.12% w/v), (c) in mesitylene (0.21% w/v).(d) in chloro benzene (0.2% w/v)

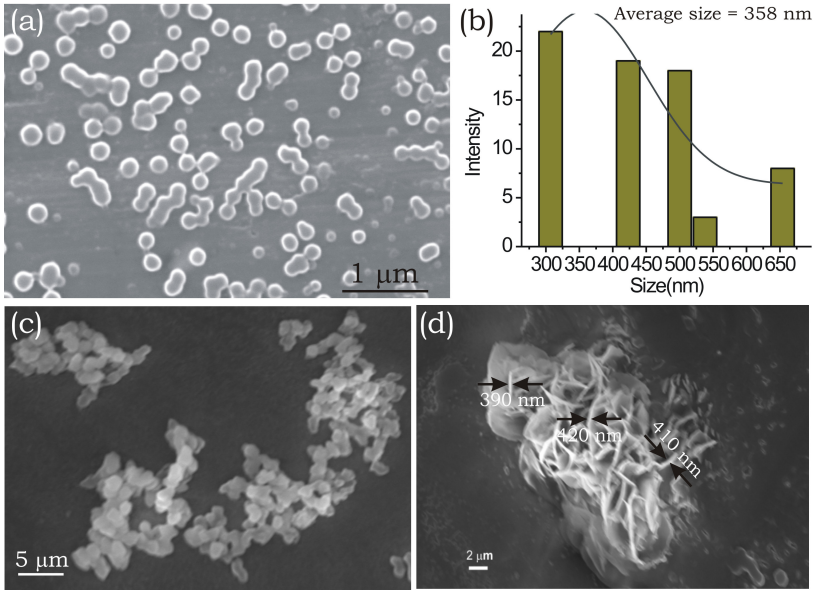

Fig. S7: Scanning electron micrographs of dried self-assemblies of ursolic acid in m-xylene: (a) 0.23 % (w/v), (b) histogram of (a), (c) 0.52 % (w/v), (d) 0.52 % (w/v).

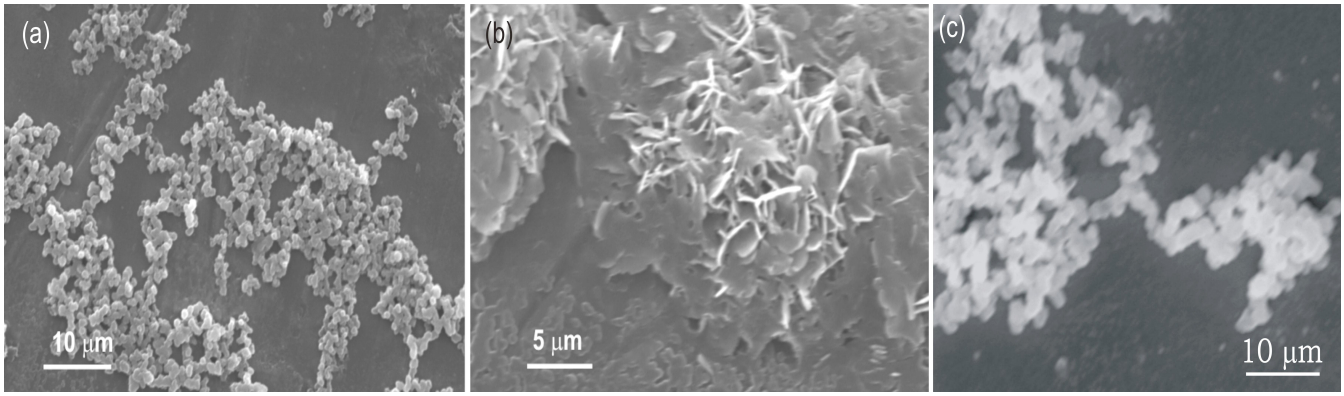

Fig. S8: (a,b) Scanning electron micrographs of the dried self-assemblies of ursolic acid in toluene (1.0% w/v), (c) Scanning electron micrographs of the dried self-assemblies of ursolic acid in mesitylene (1.4% w/v).

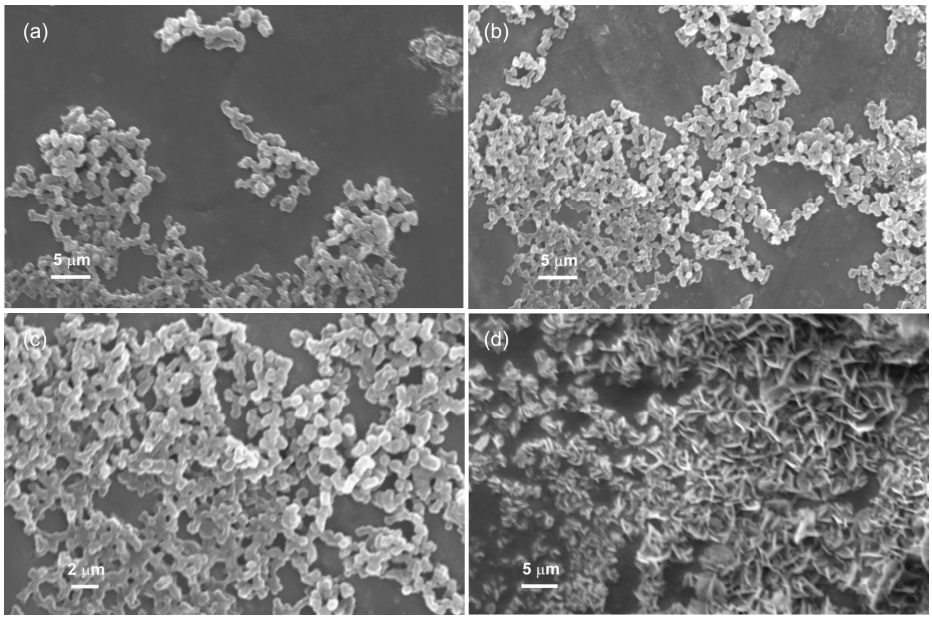

Fig. S9: (a-d) Scanning electron micrographs of the dried self-assemblies of ursolic acid **1** in chlorobenzene (1.04% w/v).

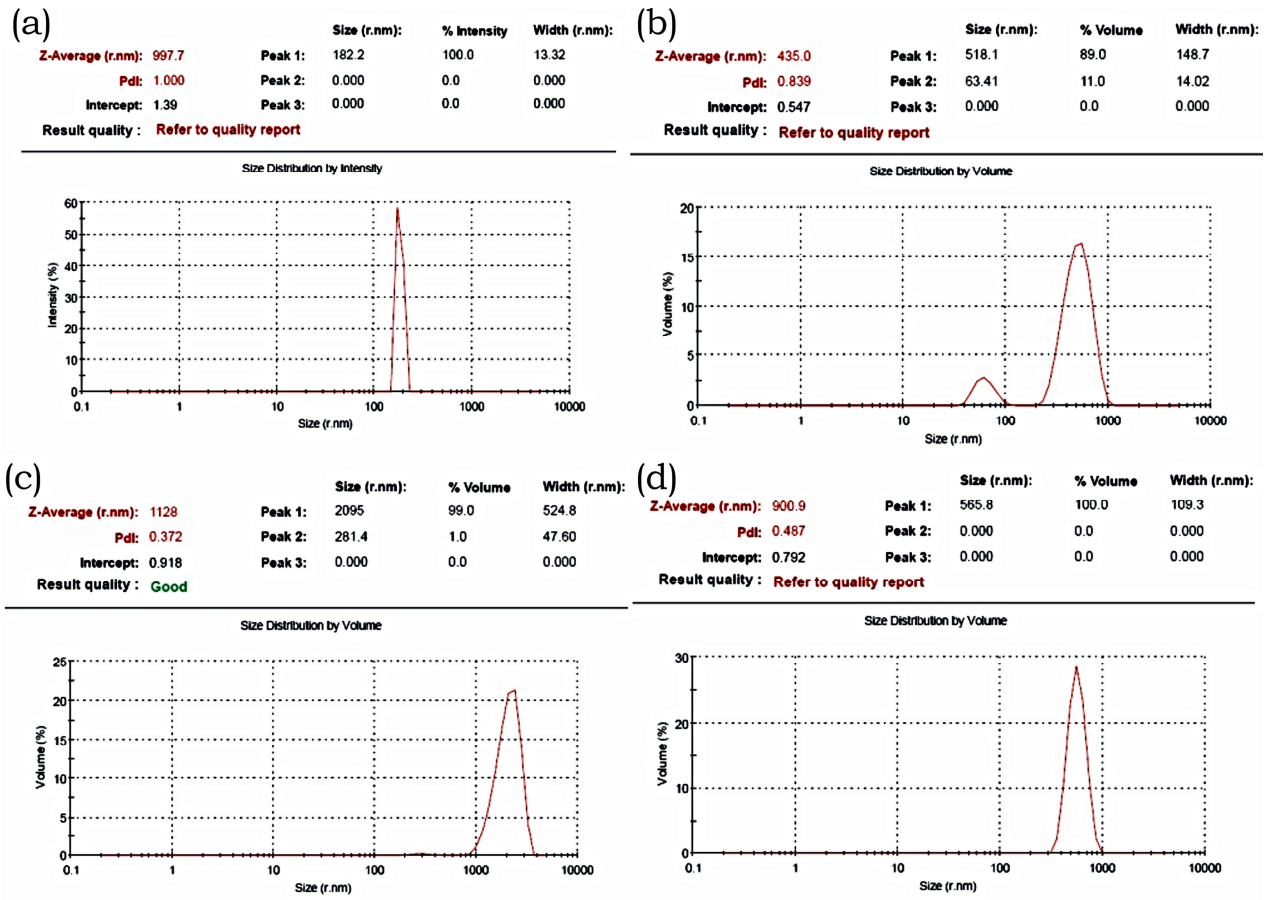

Fig.S10: Dynamic light scattering (DLS) studies of **1** in : (a) ethanol- water (0.23% w/v); (b) o-dichlorobenzene (0.16% w/v); (c) chloro benzene (0.2% w/v); (d) mesitylene (0.21% w/v).

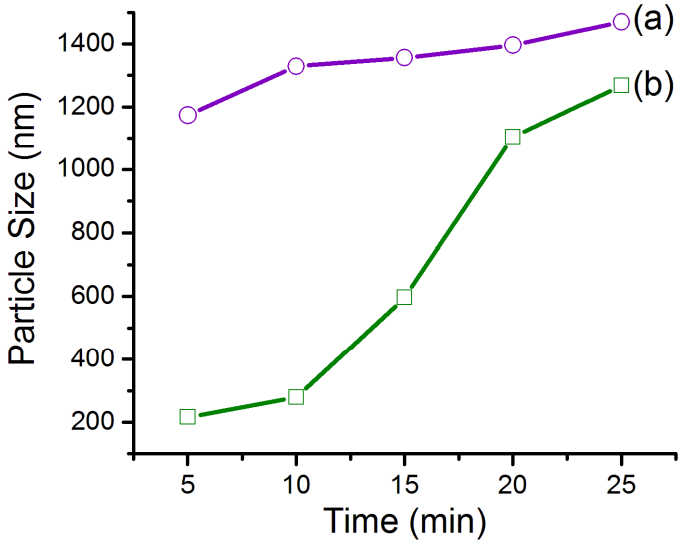

Fig. S11: Particle Size vs time plot by dynamic light scattering (DLS) studies of **1** in : (a) DMSO- water (0.08 % w/v); (b) DMSO- water (0.05 % w/v).

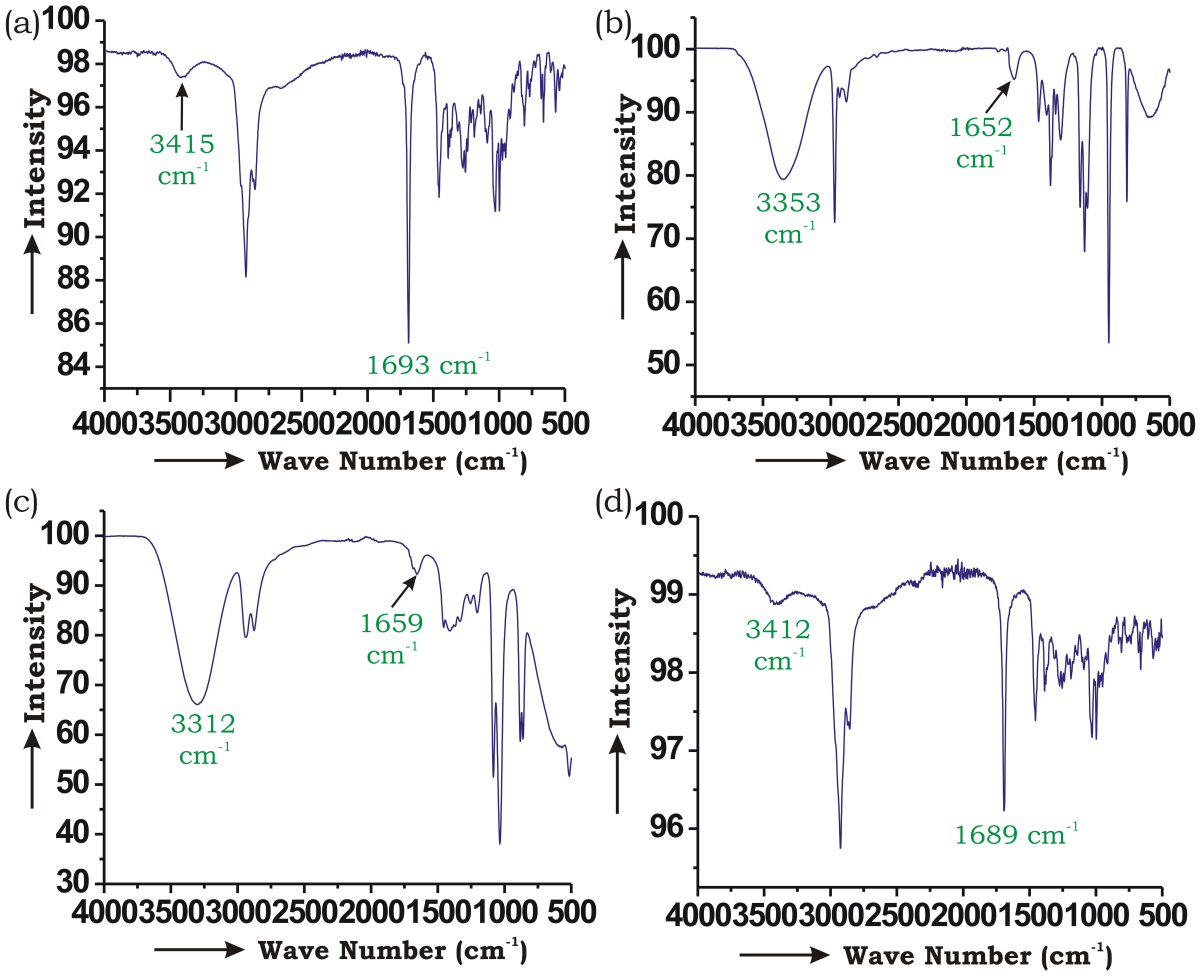

Fig. S12: ATIR studies of Ursolic Acid (a) and its dried self-assemblies in (b) iso-propylalchol; (c) 0-dichlorobenzene; (C) PhBr.

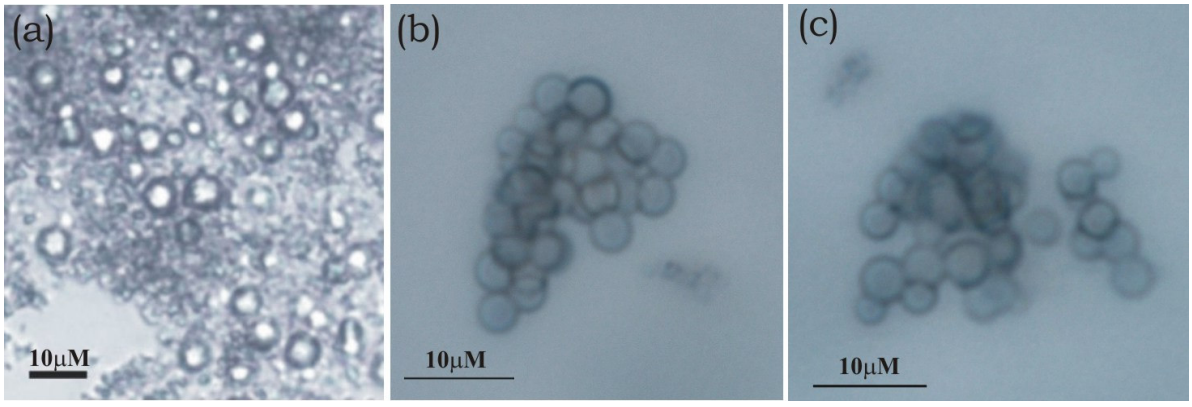

Fig. S13: Optical Microscopy image of **1**: (a) in ethanol-water (3:1, 1.3 % w/v) (b,c) in DMF-H_2O (5:1, 3.5 % w/v).

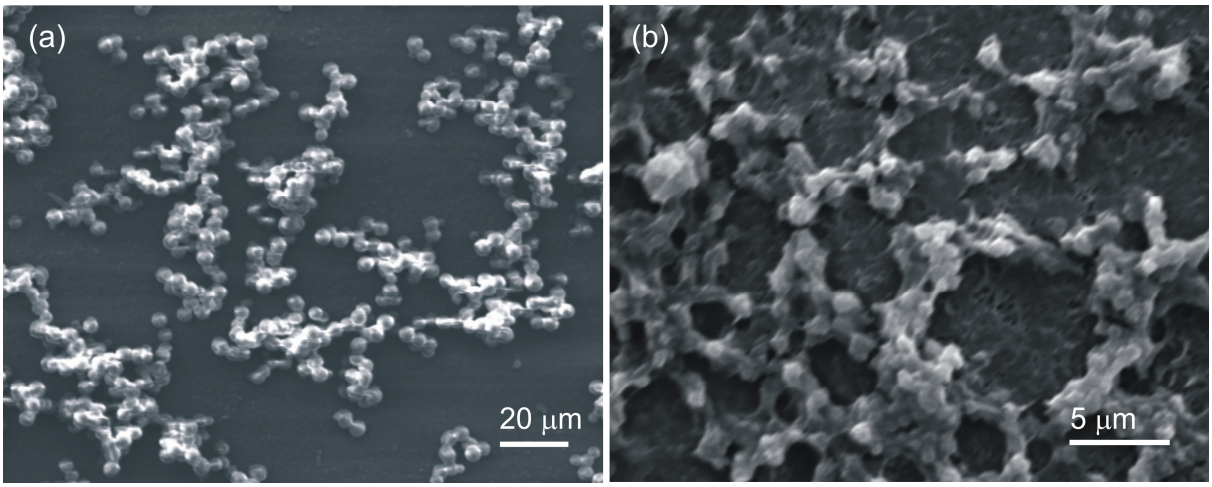

Fig. S14: Scanning electron micrographs of the dried self-assemblies of ursolic acid **1** entrapped: (a) fluorophores Rho-B in ethanol- water (1.1 % w/v), (b) anticancer drug doxorubicin in ethanol- water (0.53 % w/v).