Electronic Supplementary Information (ESI)

Carbon Dots Functionalized Gold Nanorod Mediated Delivery of Doxorubicin: Tri-functional nano-worms for Drug delivery, Photothermal therapy and Bioimaging

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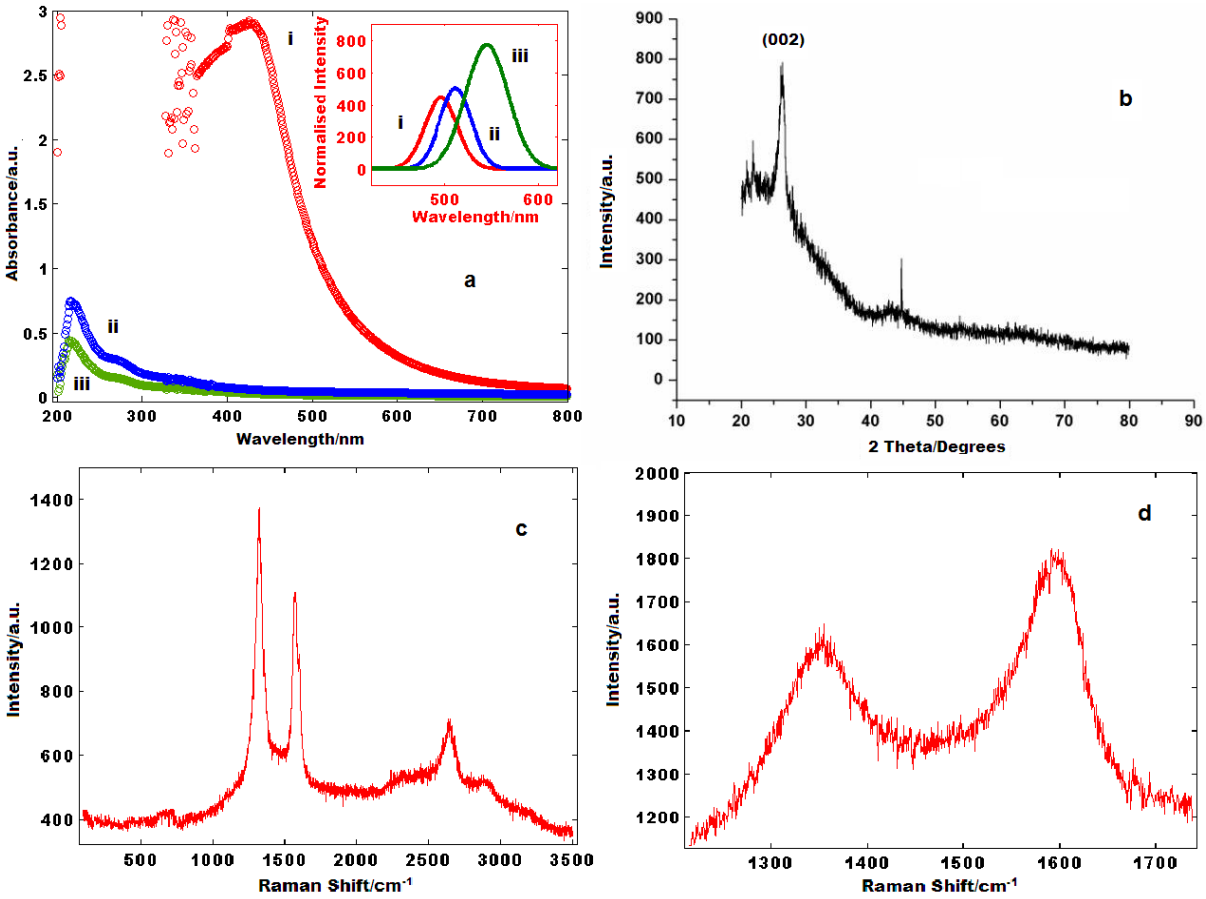

Figure S1 (a) UV-Vis Spectra of fractions F1 (i), F2 (ii) and F3 (iii) Inset shows corresponding fluorescence spectra of fractions in the similar order (b) XRD representing all the three fractions (c) Typical Raman Spectra of F1 and (d) F3.

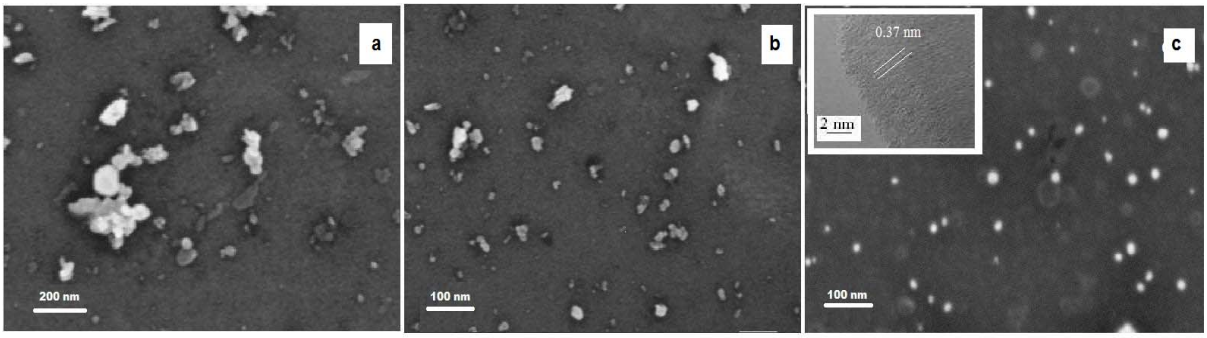

Figure S2 FEG SEM image of fractions (a) F1 showing presence of distorted GO (b) F2 showing GO with some extent of C-dots and (c) F3 showing presence C-dots. Inset shows HRTEM image of C-dots with typical lattice constant of 0.37 nm.

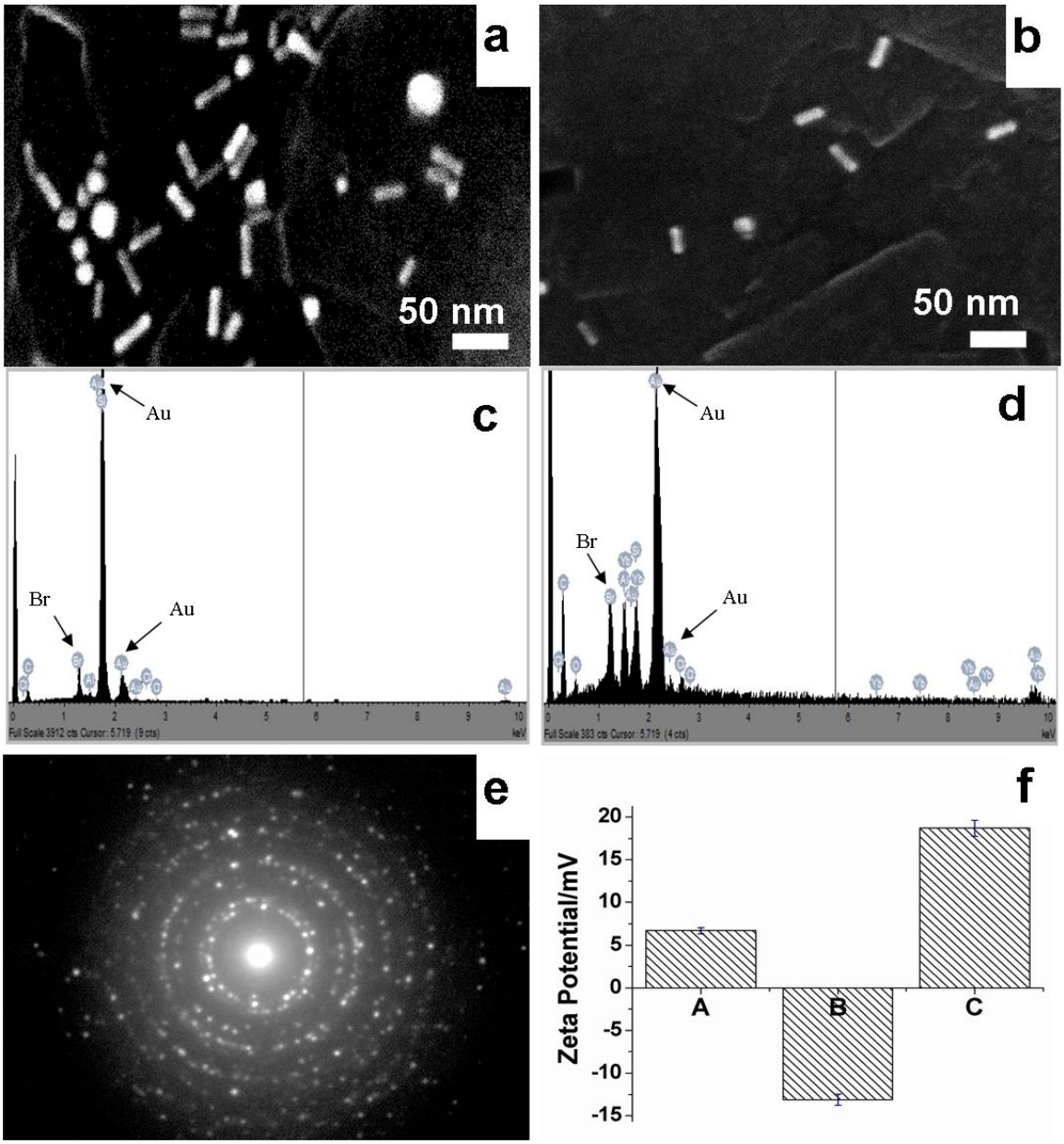

Figure S3 FEG-SEM micrographs of (a) C-dots@GNR with an average aspect ratio 2.33 (b) bare GNRs with an average aspect ratio 2.95; EDAX spectrum of (c) C-dots@GNR-DOX (d) bare GNRs, SAED pattern of (e) C-dots@GNR-DOX and (e) Zeta potential of A:GNRs, B:C-dots@GNR and C:C-dots@GNR-DOX complex. Results are expressed as mean ± standard error from independents experiments conducted thrice.

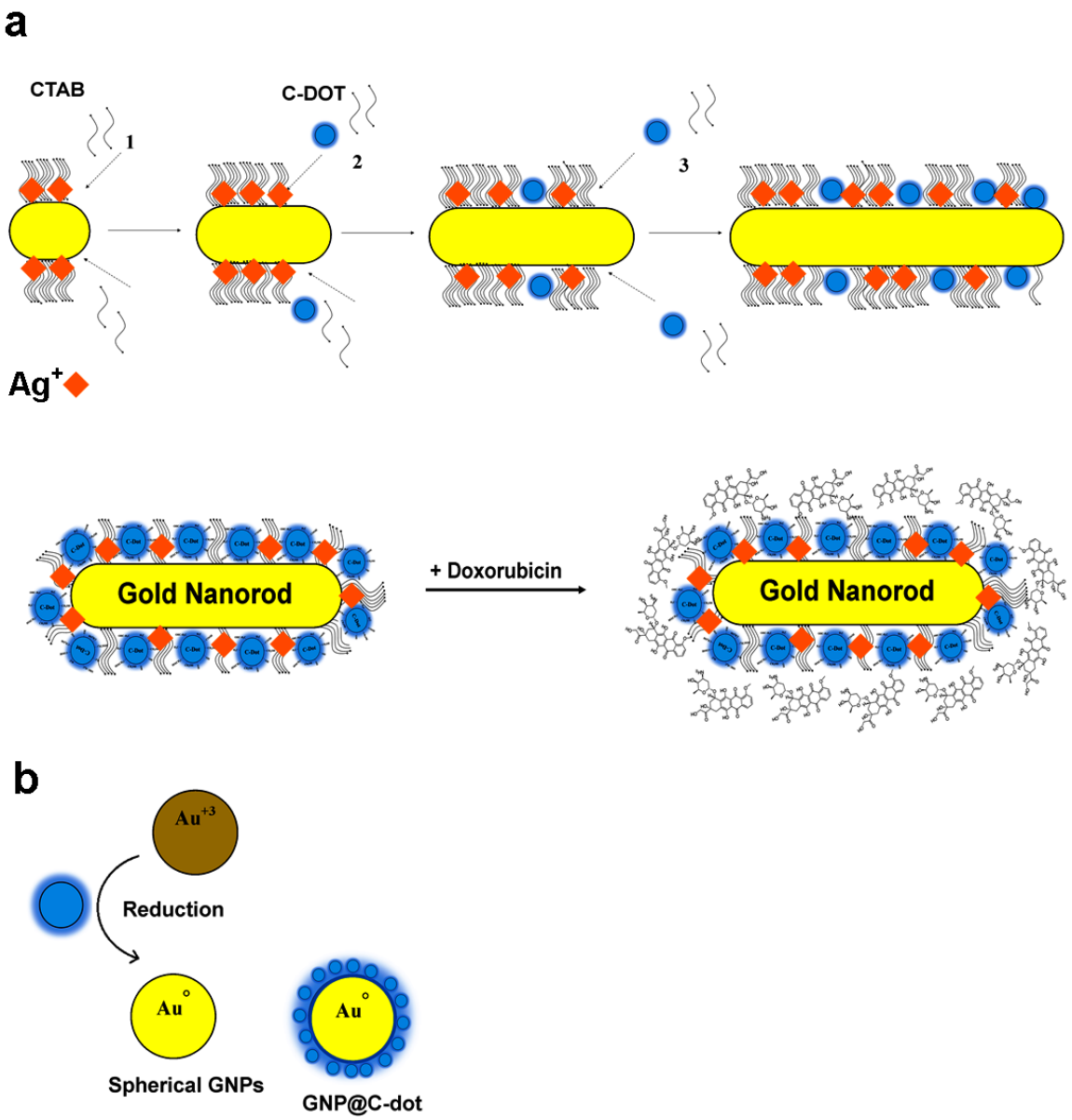

Figure S4 Schematic presentation of (a) formation C-dots@GNR complex during zipping mechanism and subsequent formation of C-dots@GNR-DOX complex and (b) synthesis of spherical gold nanoparticles coated with C-dots.

Table S1 FTIR bands and their corresponding chemical bonds:

Table S1a FTIR details of *Acacia arabica* gum extract

Sr.No.	IR Band (cm^{-1})	Representative functional groups
1.	625	C-H bend acetyl bend arising from Galactose, Arabinose, Rhamnose chains to form polysaccharides.
2.	713	Alkane CH_2 bend, alkene C-H, aromatic C-H bend due to polysaccharides, amino acids from galactoproteins.
3.	1031	Alkene C-H bend from polysaccharides.
4.	1264	Alkane CH_3 bend, Alcohol C-O stretch, Ether C-O-C stretch, carboxylic acid CO stretch, amines C-N stretch alkyl due to Sugar backbone showing alkane bend, alcohol stretch. Ether stretch is due attachment of two galactose sugars. CO and CN stretches from galactoproteins.
5.	1377	Alkane CH_3 bend, Aromatic C=C stretch, Ketone C-C stretch, carboxylic acid C-O stretch, Anhydrides C-O stretch, Amine C-N stretch from Polyssacharides, Galactoproteins.
6.	1526,1622,1683	Aromatic C=C stretch, Amide 1° N-H bend, nitro groups $-NO_2$ both aliphatic and aromatic from Galactoproteins, amino acids.
7.	2857, 2922	Sugars like Galactose, Arabinose, Rhamnose giving Alkane C-H stretch, Aldehyde C-H stretch
8.	3332	Aqueous fraction of water giving bands of alcohol OH stretch, Carboxylic acid OH stretch.

Table S1a FTIR details of carbon dots (C-dots)

Sr.No.	IR Band (cm^{-1})	Representative functional groups
1.	631, 1044	C-H acetyl bend, Alkene C-H bend (monosubstituted) saturated hydrocarbons on C-dot surface.

3.	1257	Alcohol C-O stretch, Ether C-O-C stretch, Ketone C-C stretch, carboxylic acid C-O stretch from surface functional groups passivized using NaOH.
4.	1534,1626, 1680	Aromatic C=C stretch, Amide 1° N-H bend, Aldehyde C=O stretch, Anhydride C=O stretch from polysaccharide and residual amino acid backbone.
5.	1737	Aldehyde C=O stretch, Ketone C=O stretch, Carboxylic acid C=O stretch, Anhydride C=O stretch surface passivized using NaOH.
6.	2933	Alkane C-H stretch, Aldehyde C-H stretch, Alkenes =CH stretch, Aromatic CH stretch, Carboxylic acid OH stretch, Amide NH stretch polysaccharide carbon backbone.
7.	3337	Alcohol OH stretch, Carboxylic acid OH stretch due to aqueous solution.

Table S1c FTIR details of gold nanorods (GNRs)

Sr.No.	**IR Band (cm^{-1})**	**Representative functional groups**
1.	668	Alkane CH_2 bend from CTAB associated with GNRs backbone and alkyl halide C-Br stretch which may arise due to from terminal attachment with quaternary ammonium (arsing from CTAB) from one molecule to methyl group of other CTAB molecule.
2.	1462, 1554	Alkane CH_3 bend from hydrophobic core of CTAB backbone linked to GNRs
4.	1641	Alkene C=C stretch isolated and conjugated, Aromatic C=C stretch, Amine N-H bend, Amide C=O stretch and NH bend, Imines R_2C=NR stretch
5.	2852, 2921	Carboxylic acids OH stretch Amide NH stretch from hydrogen bonding between aqueous suspension and CTAB.
6.	3450, 3744	Alcohol O-H stretch, Carboxylic acid OH stretch of aqueous suspension.

Table S1d FTIR details of C-Dots@GNR conjugate

Sr.No.	IR Band (cm^{-1})	Representative functional groups
1.	556	Alkyl halide CBr stretch from gold nanorods linked with CTAB , Alkane CH_2 bend from surfactant hydrophobic chain
2.	856	Acid chloride (C-Cl) due to interaction of chloride from gum extract with GNRs and C-dot complex
3.	93, 1051	Alkenes CH bend, Anhydride C-O stretch
4.	1132, 1417, 1644	Alkane CH_3 bend, Alcohol C-O stretch, Ether C-O-C stretch, Ketone C-C stretch, carboxylic acid C-O stretch, Ester C-C(O)-C acetate, amines C-N stretch alkyl, Sulfones S=O stretch, Phosphine PH bend, Phosphine oxides P=O
5.	2928	Alkane C-H stretch, Aldehyde C-H stretch, Carboxylic acid OH stretch from surface passivized C-dots
6.	3417	Alcohol O-H stretch, Carboxylic acid OH stretch from aqueous suspension.

Table S1e FTIR details of DOX

Sr.No.	IR Band (cm^{-1})	Representative functional groups
1.	614	Aromatic CH bend from hydrophobic benzene rings
2.	703, 1435, 1661	Alkane CH_2 bend, alkene C-H, aromatic C-H bend (meta),acid chloride (C-Cl)
3.	952, 1028, 1317, 1661	Alkenes CH bend, Anhydride C-O stretch, Amine C-N stretch
4.	2917	Alkane C-H stretch, Aldehyde C-H stretch, Alkenes =CH stretch, Aromatic CH stretch, Carboxylic acid OH stretch, Amide NH stretch

5.	3000, 3459, 3780	Alkane C-H stretch, Aldehyde C-H stretch, Alkenes =CH stretch, Aromatic CH stretch, Carboxylic acid OH stretch, Amide NH stretch

Table S1f FTIR details of C-dot@GNR-DOX complex

Sr.No.	**IR Band (cm^{-1})**	**Representative functional groups**
1.	428	Alkyl halide CBr stretch during the formation of the conjugate
2.	605	Alkane CH_2 bend, Alkene CH bend, Alkyne acetylenic CH bend, Aromatic CH bend
3.	700, 1020	Alkane CH_2 bend, alkene C-H, aromatic C-H bend (meta),acid chloride (C-Cl)
5.	1437, 1590	Aromatic C=C stretch, Carboxylic acids OH bend from doxorubicin structure
6.	2923	Alkenes =CH stretch, Aromatic CH stretch, Amide NH stretch due to interaction between C-dot surface and doxorubicin
7.	3505, 3786	Aqueous suspension

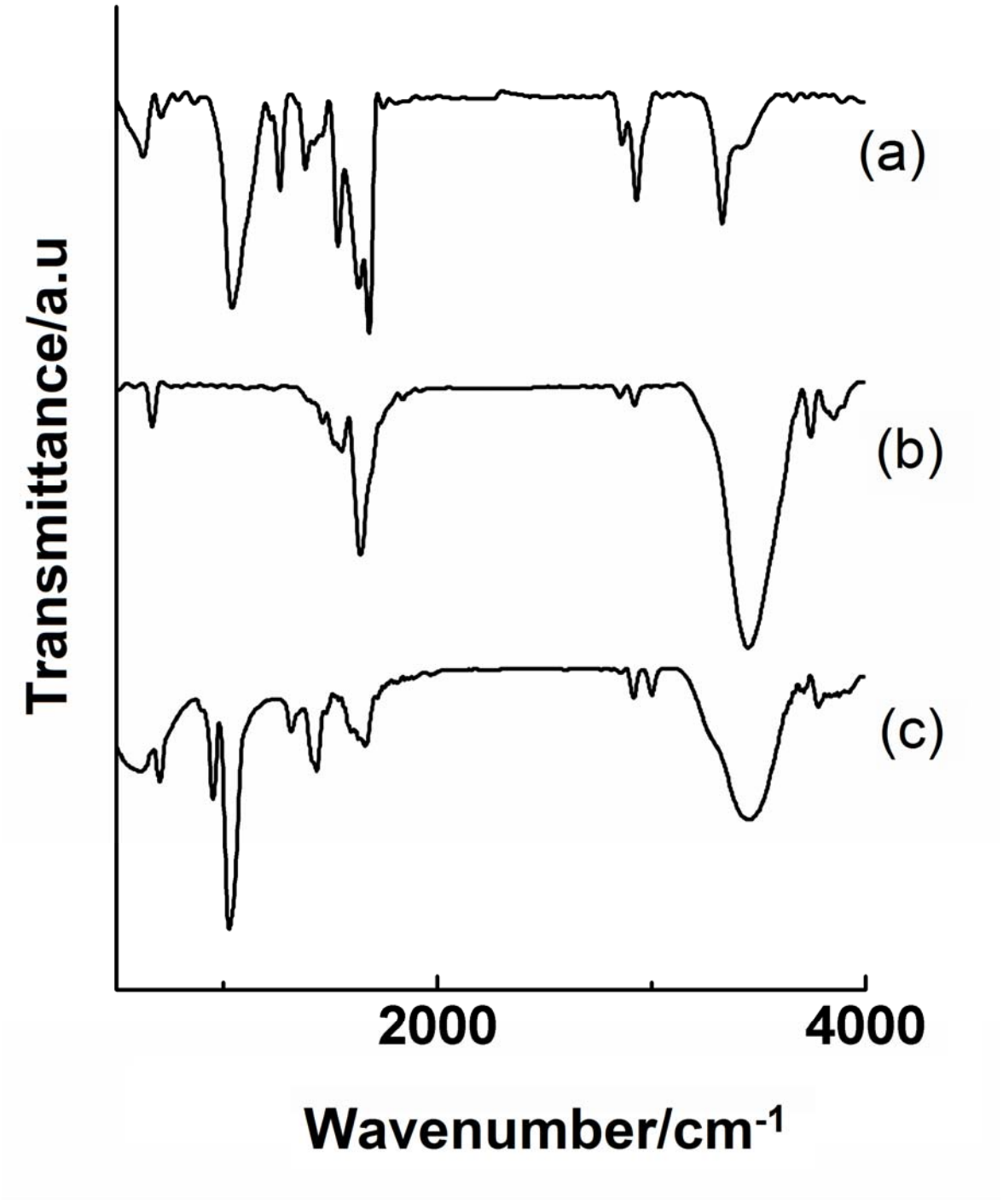

Figure S5 FTIR spectra of (a) Acacia arabica gum extract used to prepare C-dots, (b) bare GNRs and (c) free doxorubicin (DOX).

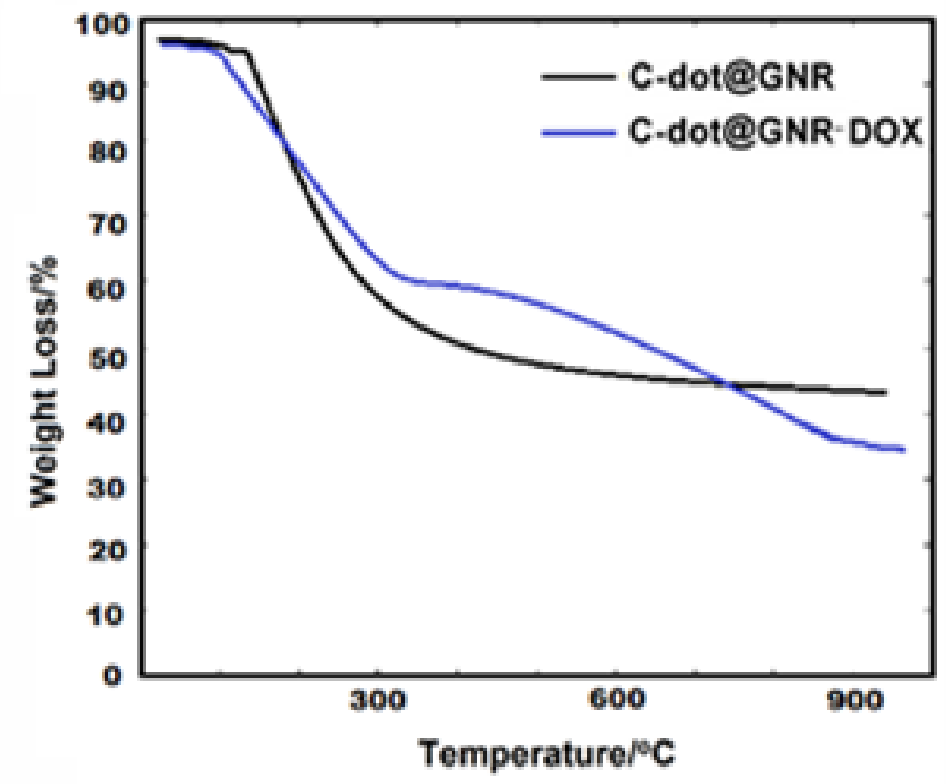

Figure S6 Thermo gravimetric analysis (TGA) measurement of C-dots@GNR and C-dots@GNR-DOX complex.

Scheme S1 Calculation for Drug loading Efficiency

Concentration of drug initially loaded= 0.0625 mM

Concentration of unbound drug= 0.0037 mM

[Concentration of drug is calculated using the standard calibration curve of DOX (Straight line equation: y=6.721x)]

Concentration of drug loaded= [Concentration of drug initially loaded] – [Concentration of drug of unbound drug]

= 0.0625 mM – 0.0037 mM

= 0.0588 mM

Drug Loading Efficiency (%) = (Concentration of drug finally loaded/Concentration of drug initially loaded)*100

= 0.0588/0.0625*100

= 94.08 %