Electronic Supplementary Material (ESI) for RSC Advances.

One-Step Synthesis of Silver Metallosurfactant as Efficient Antibacterial and Anticancer Material

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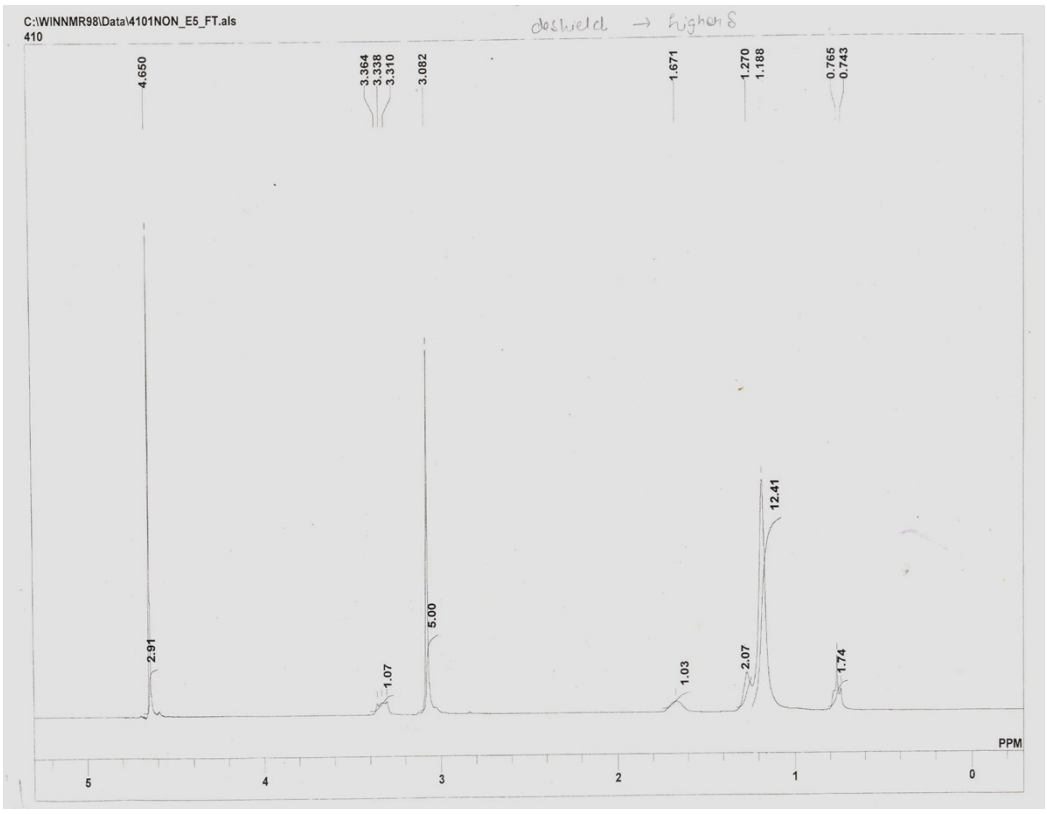
Supplement Material

Table S1: Vibrational bands for CTAB and CTA-AgB

Functional group	pure CTAB (cm^{-1})	Ag-CTAB (cm^{-1})	Br-Ag
-CH_2- sym stretching	2915.46, 2848.12	2848.12, 2914.14	
-Asymmetric and symmetric CH scissoring vibrations of CH_3-N^+	1484, 1472.75	1484.18, 1463.9	
N-C sym stretching of N-$(CH_3)_3$- moiety	1407.35, 1382.35, 1258.12	1332.69	
Rocking mode of methylene chain	729.9, 718.5	718.7	
Br-Ag	------	-----	215, 170, 49
N-Br-Ag	----	231, 112	

Table S2: Chemical shifts of CTAB and CTA-AgB

group	δ_{CTAB}	$\delta_{CTAB-Ag}$	$\Delta\delta$
α-CH_3	3.082	3.002	0.080
α'-CH_2	3.338	3.205	0.133
β'-CH_2	1.671	1.635	0.036
β-CH_2	1.270	1.232	0.038
γ'- CH_2	1.188	1.172	0.016
γ-CH_3	0.765	0.754	0.011



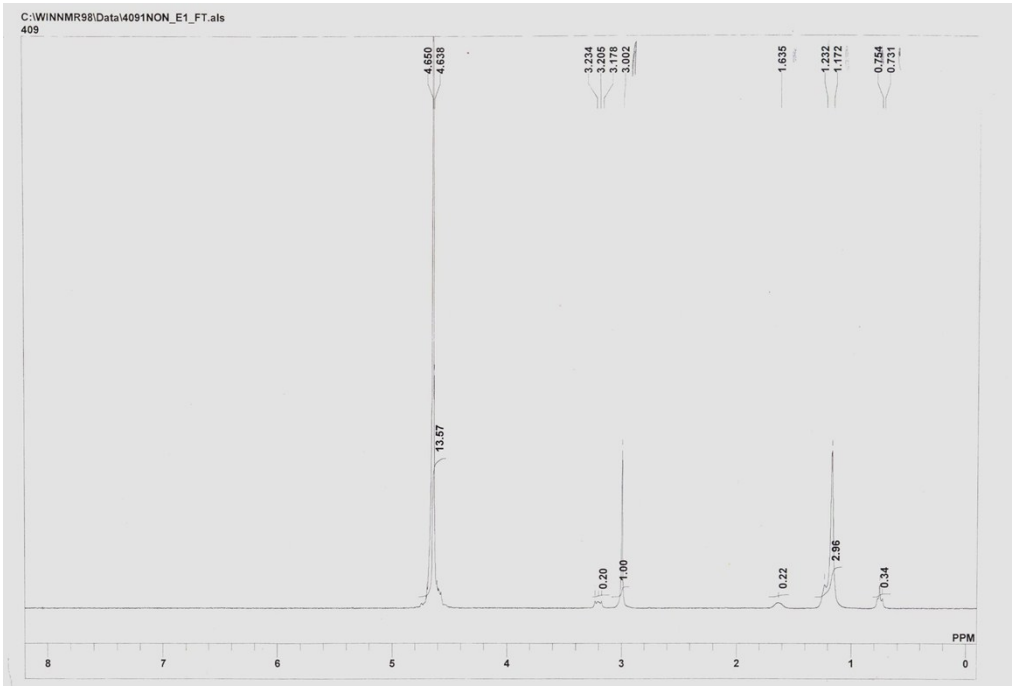


Figure S1: [1]HNMR of (a) CTAB (b) CTA-AgB

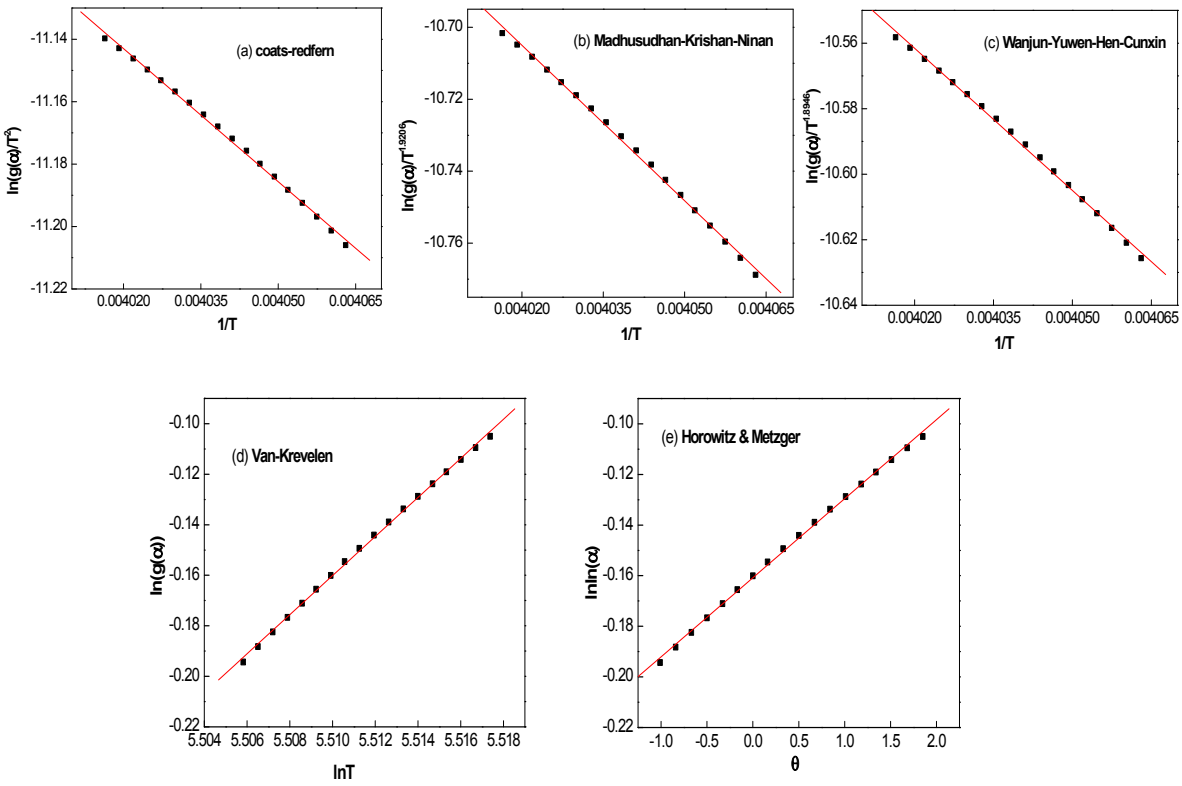


Figure S2: Linearisation curves obtained by (a) Coats–Redfern (CR), (b) Madhusudanan-Krishnan–Ninan (MKN), (c) Wanjun–Yuwen–Hen–Cunxin (WYHC), (d) van Krevelen (vK) methods and (e) Horowitz–Metzger (HM) methods for CTAB

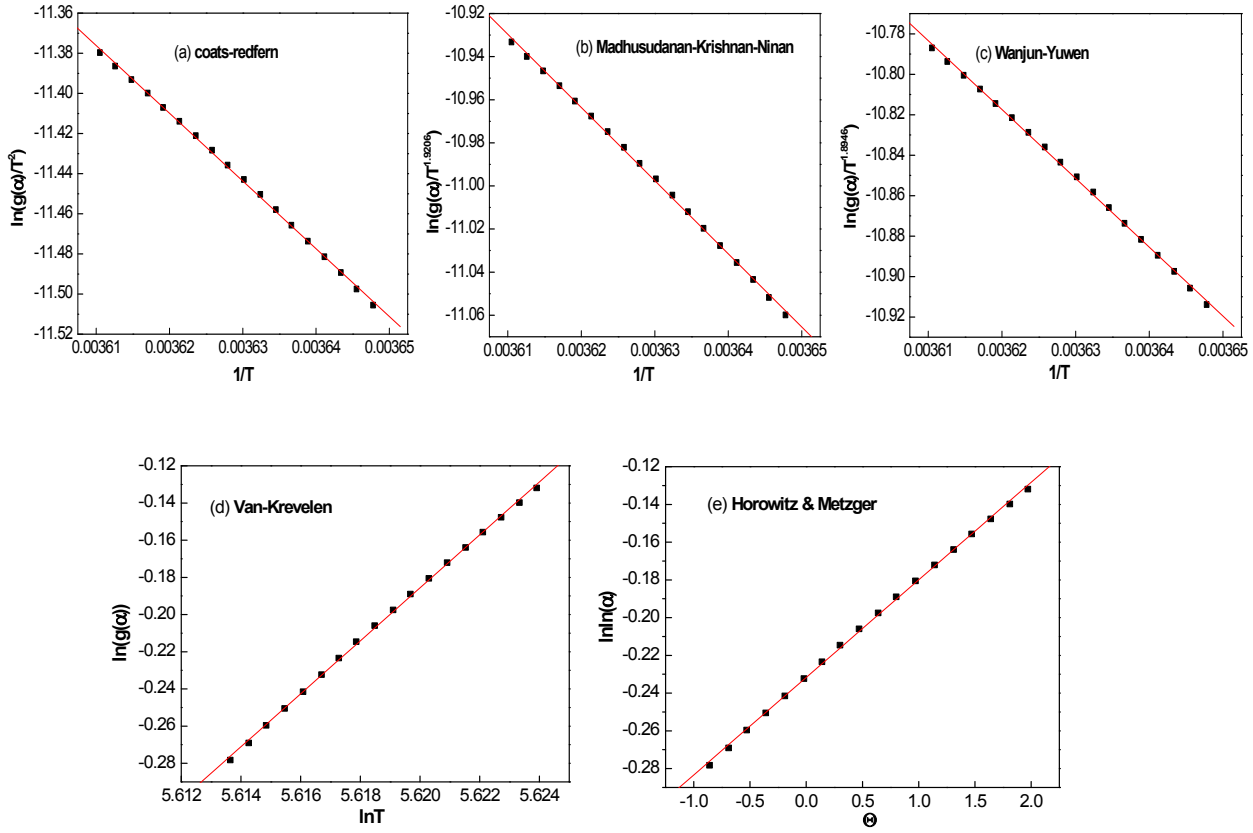


Figure S3: Linearisation curves obtained by (a) Coats–Redfern (CR), (b) Madhusudanan-Krishnan–Ninan (MKN), (c) Wanjun–Yuwen–Hen–Cunxin (WYHC), (d) van Krevelen (vK) methods and (e) Horowitz–Metzger (HM) methods for CTA-AgB

Thermodynamics of micellization

Thermodynamic parameters such as ΔG_m^o (Gibbs free energy), ΔH_m^o (enthalpy) and ΔS_m^o (entropy) of micelle formation have been estimated using following equations

$$\Delta G_m^o = (2-\beta)RT \ln X_{cmc} \quad \text{(S1)}$$

$$\Delta H_m^o = -RT^2(2-\beta)d\ln X_{cmc}/dt \quad \text{(S2)}$$

$$\Delta S_m^o = (\Delta H_m^o - \Delta G_m^o)/T \quad \text{(S3)}$$

where, R, T, β and X_{cmc} represents gas constant, absolute temperature, degree of ionization and cmc in terms of mole fraction, respectively.

Table S3: cmc, surfactant ionization parameter (β) and thermodynamic parameters of micellization of CTA-AgB

Temp (K)	CTAB cmc (mM)	CTA-AgB cmc (mM)	β	$\ln X_{cmc}$	ΔG_m^o (kJ mol^{-1})	ΔH_m^o (kJ mol^{-1})	ΔS_m^o (kJ mol^{-1} K^{-1})
298.15	0.84-0.97[39,40]	1.02	0.35	-10.90	-44.42	-18.56	0.087
303.15	1.10	1.08	0.40	-10.85	-43.73	-18.66	0.083
308.15	1.21	1.17	0.41	-10.77	-43.65	-19.07	0.079
313.15	1.35	1.27	0.43	-10.68	-43.59	-19.50	0.076

where, $\ln X_{cmc}$ is cmc in terms of mole fraction

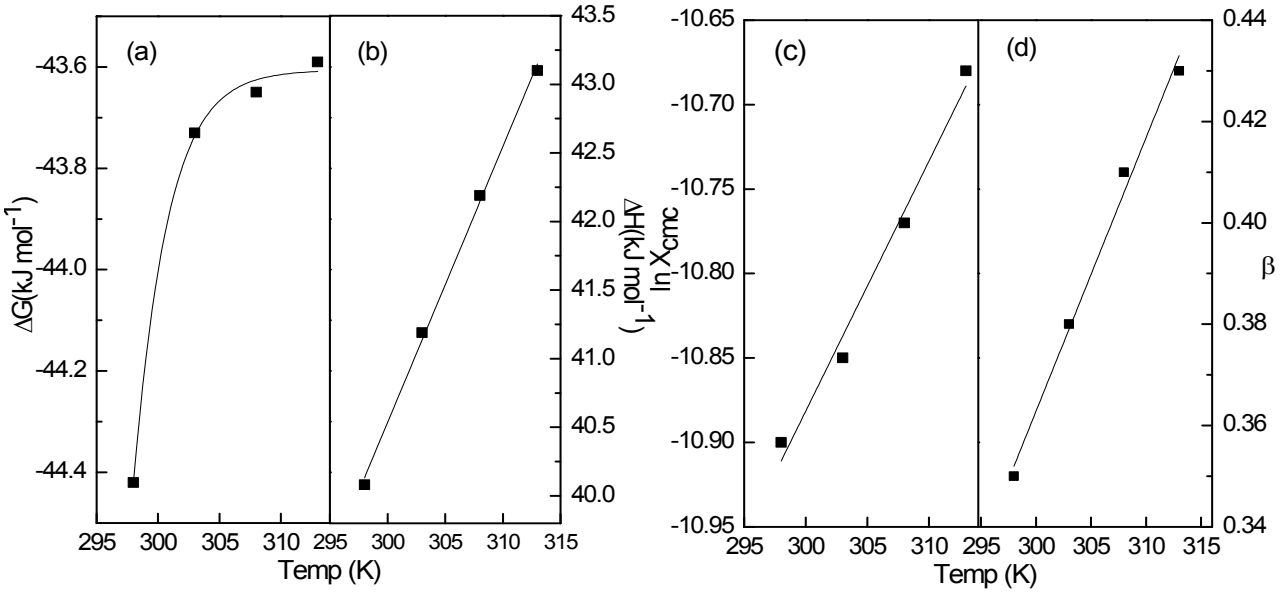


Figure S4: Variation of (a) ΔG^{o}_{m} (b) ΔH^{o}_{m} (c) ln X_{cmc} (d) β of CTA-AgB with temperature.

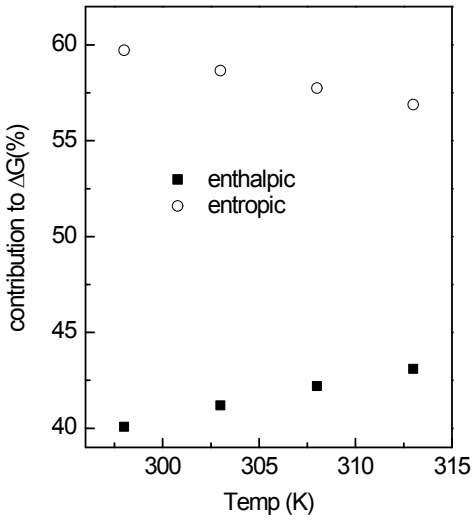


Figure S5**:** Enthalpic and entropic contributions to ΔG^{o}_{m} for CTA-AgB surfactant.

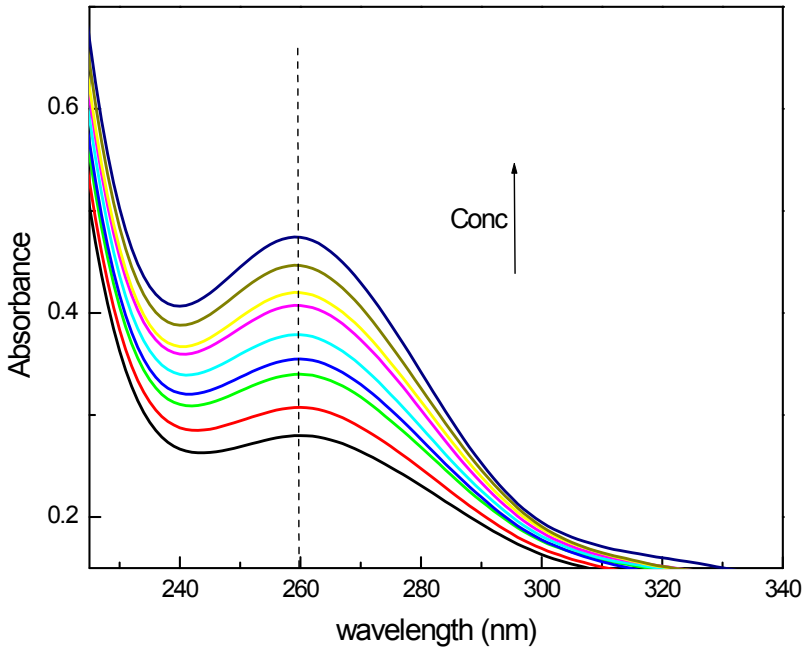


Figure S6**:** UV-visible spectra of DNA alone with increasing

Table S4: Average zone of inhibition against different microbes

Microbes	Average zone of inhibition (in mm) at dose of 0.5mg/mL	Colony formation at various dilutions of 0.5 mg/mL				
		$0.5X10^{-1}$	$0.5X10^{-2}$	$0.5X10^{-3}$	$0.5X10^{-4}$	$0.5X10^{-5}$
E. coli	11	0	60	C	C	C
S. aureus	11	36	76	288	C	C
A. niger	11	19	21	21	39	45
A. fumigatus	11	4	6	6	8	10
C. herbarium	11	5	6	14	168	C
C. lunata	12	96	232	302	504	C
H. oryzae	10	30	72	100	116	C