Supporting Information

N,N'-dialkylcystinegemini and monomeric N-alkyl cysteine surfactants as corrosion inhibitors on mild steel corrosion in 1M HCl solution – a comparative study

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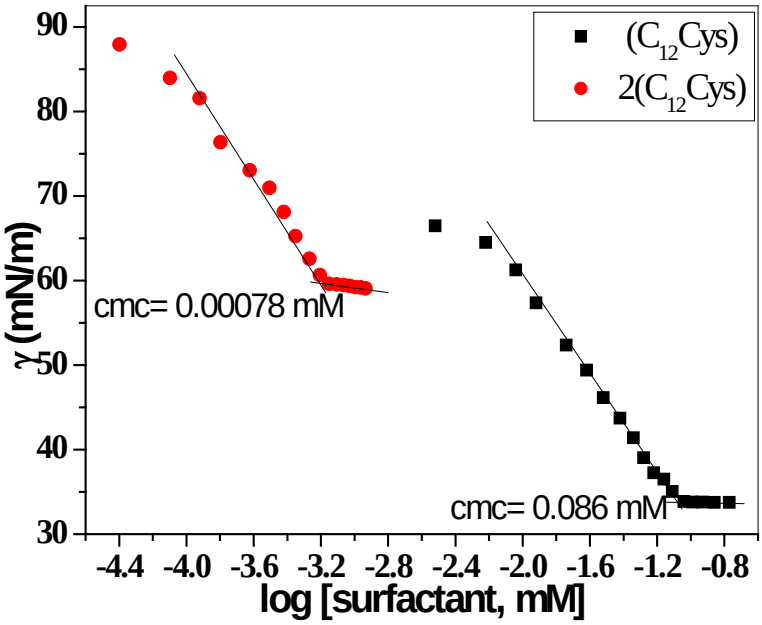


Figure S1. Variation in surface tension vs. concentration for (C_{12}Cys) and 2(C_{12}Cys).

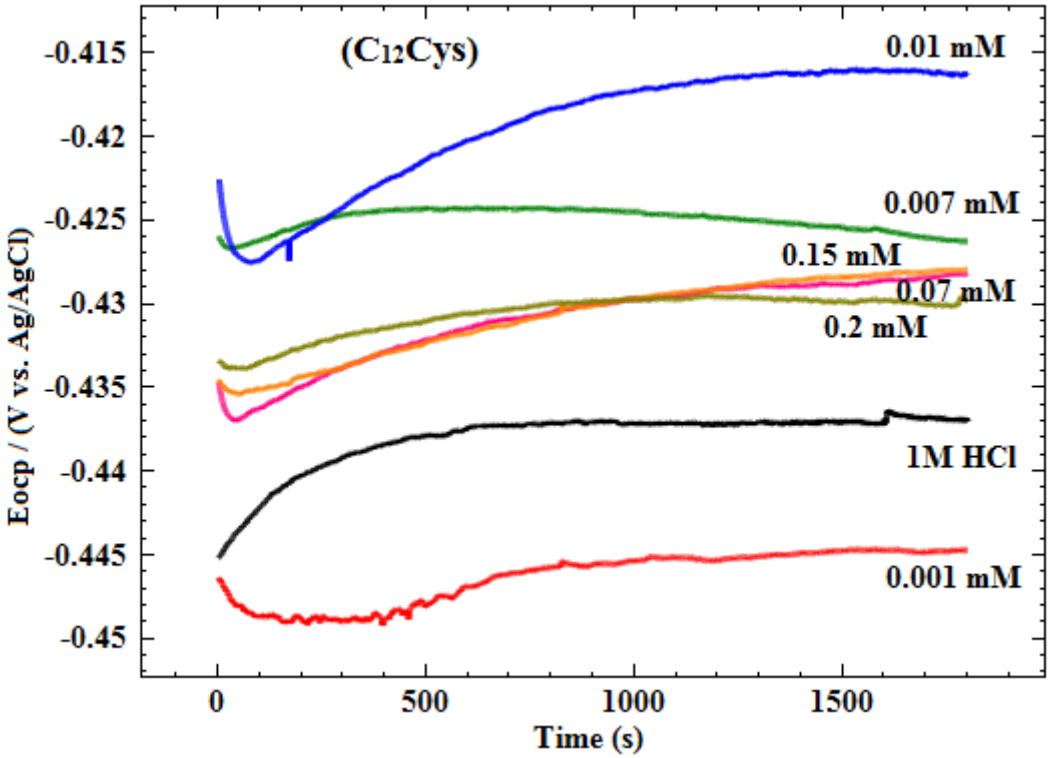


Figure S2. Variation of E_{OCP}-time curves for MS in uninhibited and inhibited 1M HCl solution (temperature 303±2 K).

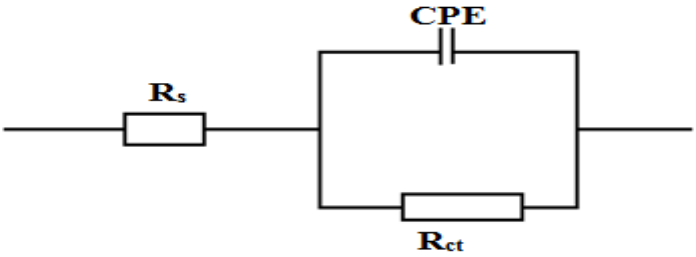


Figure S3. Randles equivalent circuit used to fit the impedance data.

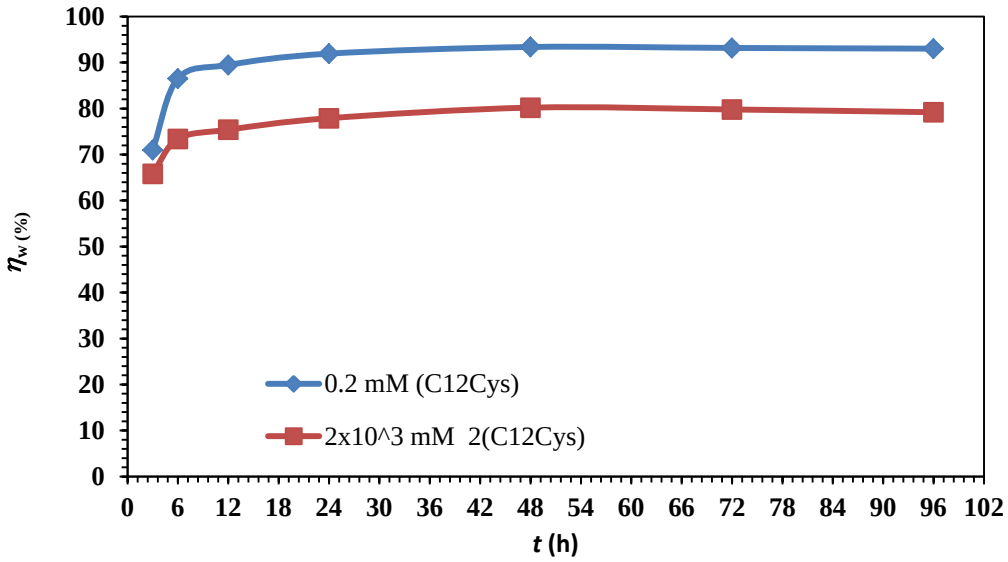
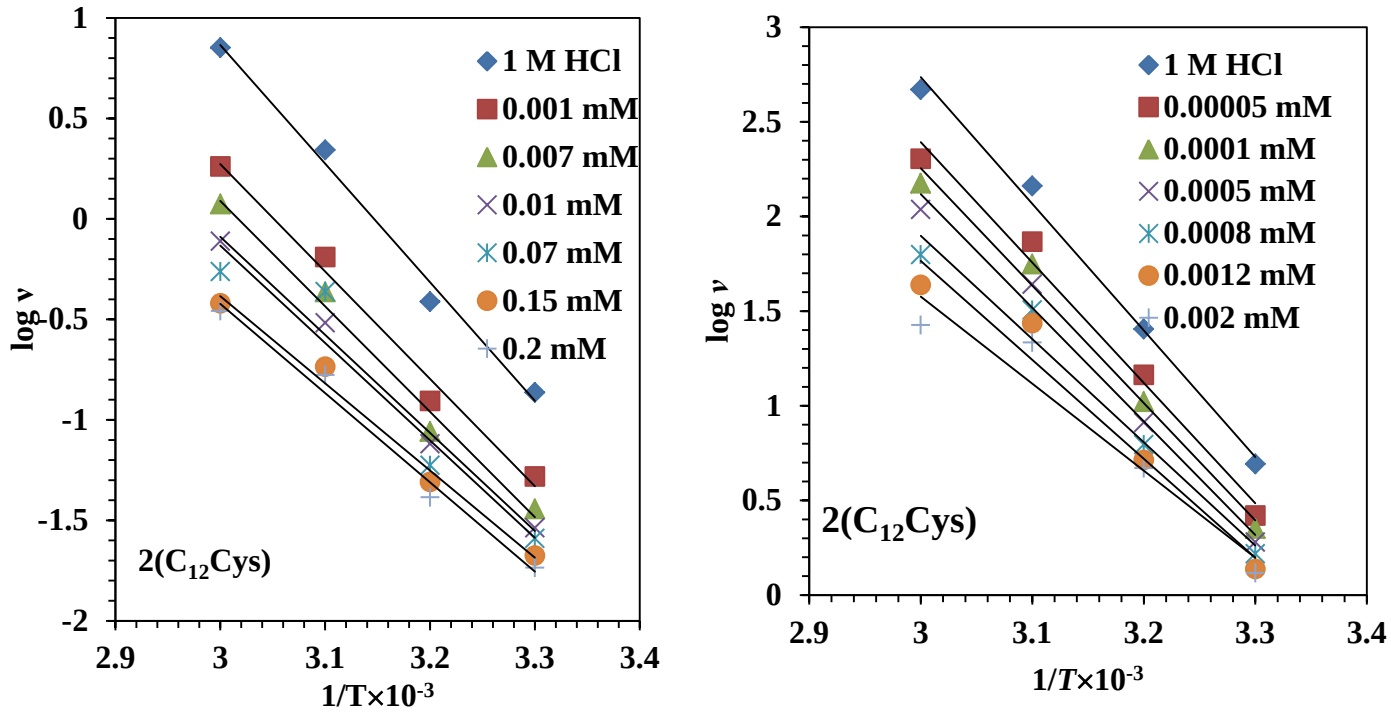
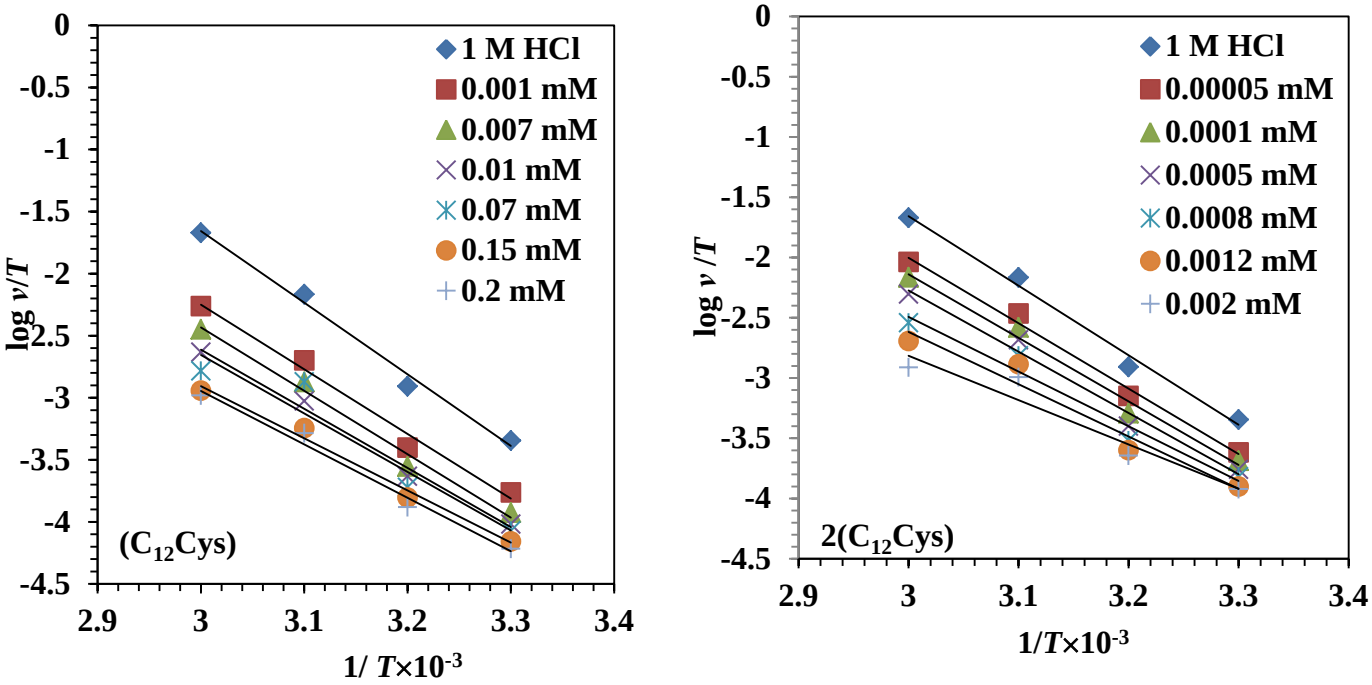


Figure S4. Variation of inhibition efficiency (η_w) with immersion time (t).



(a)



(b)

Figure S5. (a) Arrhenius plots for MS in 1M HCl in the absence and presence of different concentrations of (C_{12}Cys) and 2(C_{12}Cys). (b) Alternative Arrhenius plots for MS in 1 M HCl in the absence and presence of different concentrations of (C_{12}Cys) and 2(C_{12}Cys).

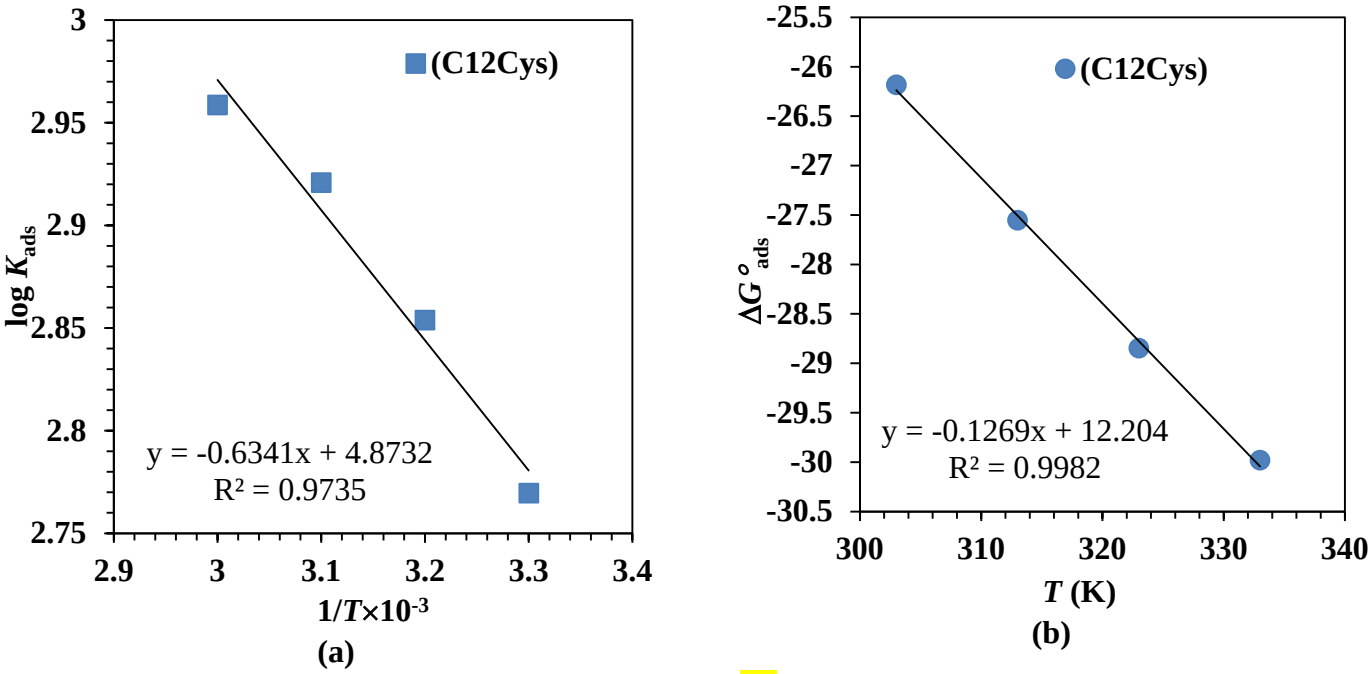


Figure S6. (a) Linear regression between log K_{ads} vs. $1/T$ (b) verification plot of $\Delta G°_{ads}$ vs. T.

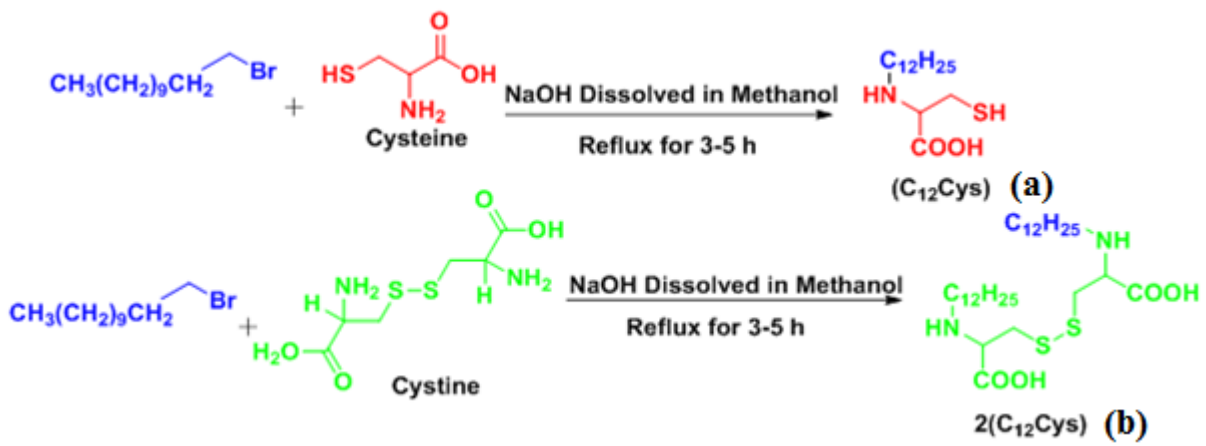
Table S1 Surface active parameters of (C_{12}Cys) and 2(C_{12}Cys) in 1M HCl solution

Inhibitor	CMC (mM)	γ_{CMC}(mN/m)	π_{CMC}(mN/m)	Γ_{max} 10^7×mol/m^2)	A_{min} (Å^2/molecule)	$\Delta G°_{mic}$ (kJ/mol)	$\Delta G°_{ads}$ (kJ/mol)
(C_{12}Cys)	0.086	59.83	11.97	9.40	176.61	-6.18	-7.45
2(C_{12}Cys)	0.0008	34.04	37.76	9.58	173.24	-18.04	-21.97

Chemical synthesis of inhibitors. (C_{12}Cys) and 2(C_{12}Cys) used in this work were synthesized and purified as reported[25]. In the typical synthesis of N-dodecyl cysteine monomeric surfactant, (C_{12}Cys) the dodecyl bromide (45.4 mol) was added to stirred solution of cysteine (41.3 mol) dissolved in methanol containing NaOH for 5 h. The mixture was refluxed and the reaction was continued until the blue colour of the solution in the presence of thymolphthalein was not changed. After the removal of solvent the residue obtained was dissolved in water and the pH was adjusted to 5.5 by adding HCl. The precipitate obtained was collected by filtration and washed many times with hexane, acetone, and methanol. The product was obtained in the form of white solid. In the synthesis of N,N'-di dodecylcystine gemini surfactant, 2(C_{12}Cys) the dodecyl bromide (45.8 mol) was added to stirred solution of cystine (20.8 mol) which was dissolved in methanol containing NaOH for 5 h. The further synthesis was continued following the procedure reported for (C_{12}Cys).The product was

obtained in the form of yellow solid. The synthesis route and structures of both the compounds are given below.

Scheme S1. Pathway for the synthesis of (a) monomeric (C_{12}Cys) and (b) gemini 2(C_{12}Cys) surfactants.



(C_{12}Cys) and 2(C_{12}Cys) are characterized by FT-IR, ^{1}H-NMR and elemental analysis, spectral data is given below.

N-alkyl cysteine monomeric surfactant, (C_{12}Cys)

FT-IR (KBr) (cm^{-1}): 3421 (NH), 2921, 2853 (C-H), 2552 (S-H), 1599 (C=O), 1470 (O-H)1056 (C-N), 719 (-CH_2)$_n$- skeletal.

^{1}H-NMR (DMSO, 500MHz): δ 0.87 (t, 6H), 1.23-1.29 (m, 18H), 1.49-1.51 (m, 2H), 2.50-2.55 (m, 2H) 2.64 (m, 2H), 3.64 (m, 1H)

Elemental analysis: Calcd. (%) C-62.28; H-10.72; N-4.89. Found (%): C-61.16; H-10.39; N-4.98.

N,N'-dialkylcystinegemini surfactant, 2(C_{12}Cys)

FT-IR (KBr) (cm^{-1}): 3419 (NH), 2923, 2852 (C-H), 1645 (C=O), 1461 (O-H) 1057 (C-N), 723 (-CH_2)$_n$- skeletal, 515 (S–S disulphide).

^{1}H-NMR (D_2O, 500 MHz): δ 0.85 (t, 6H), 1.11-1.35 (m, 36H), 1.51-1.60 (m, 4H), 2.60 (m, 4H), 2.95 (m, 4H), 3.56 (m, 2H).

Elemental analysis: Calcd. (%) C-62.25; H-10.41; N-4.86. Found (%): C-61.16; H-10.39; N-4.81.