Electronic Supplementary Information

Biferrocenyl Schiff bases as efficient corrosion inhibitors for aluminium alloy in HCl solution: a combined experimental and theoretical study

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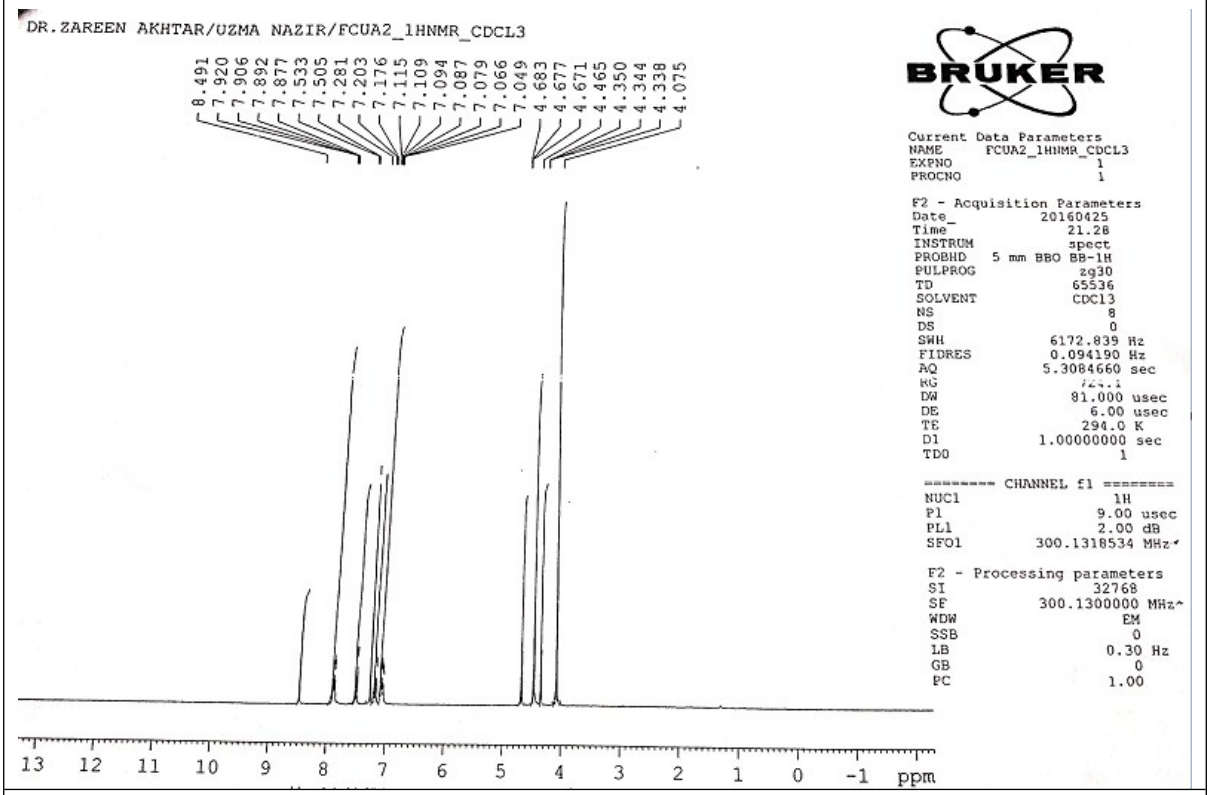

Fig. S1. ^{1}H NMR spectrum of Fcua in $CDCl_3$

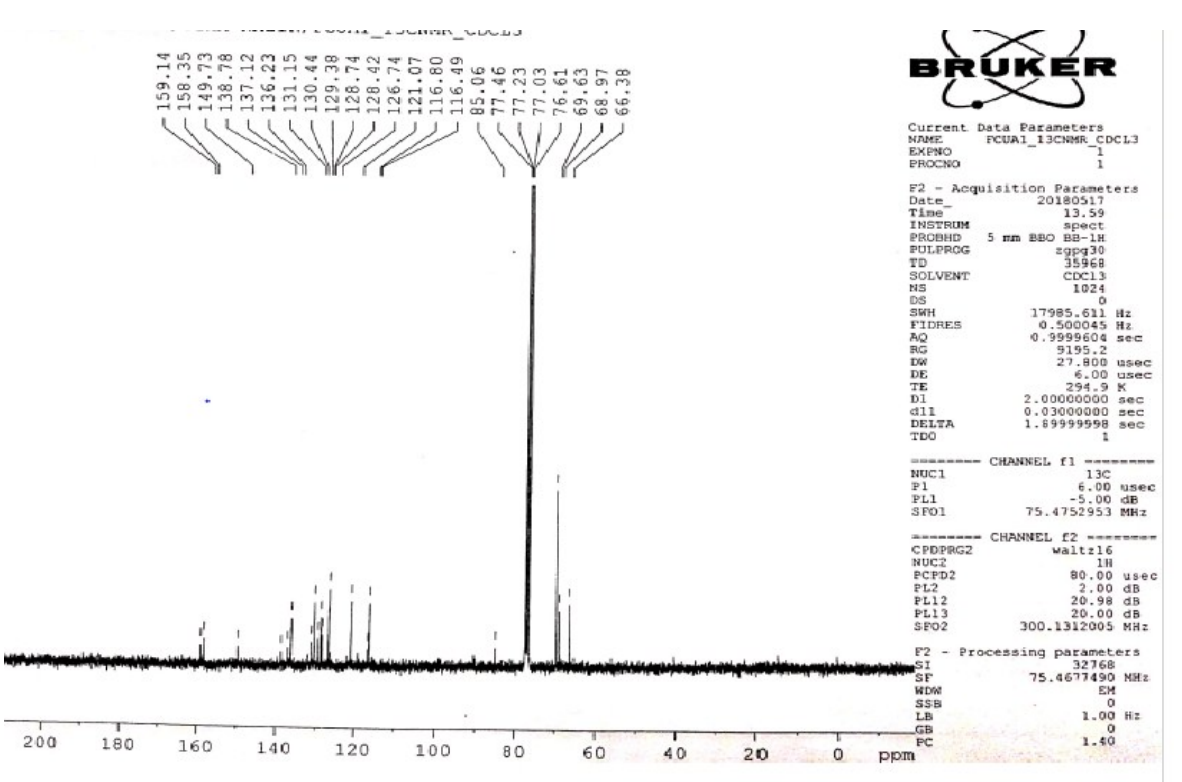

Fig. S2. ^{13}C NMR spectrum of Fcua $CDCl_3$

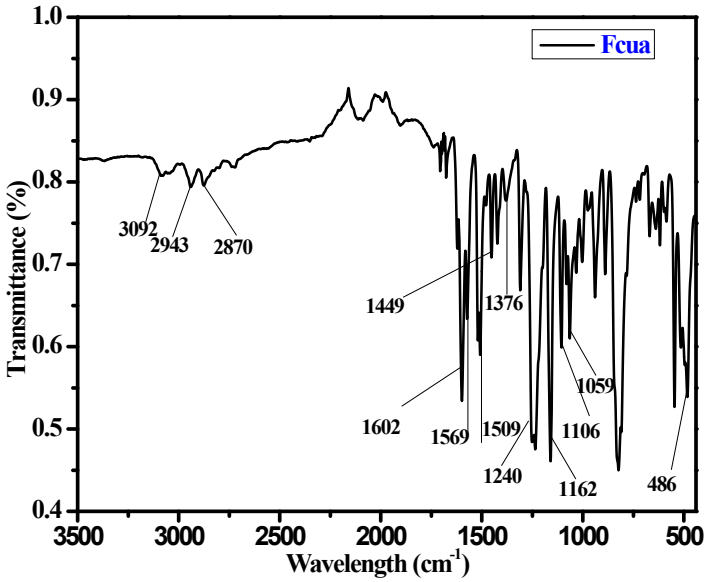

Fig. S3. FT-IR spectrum of Fcua

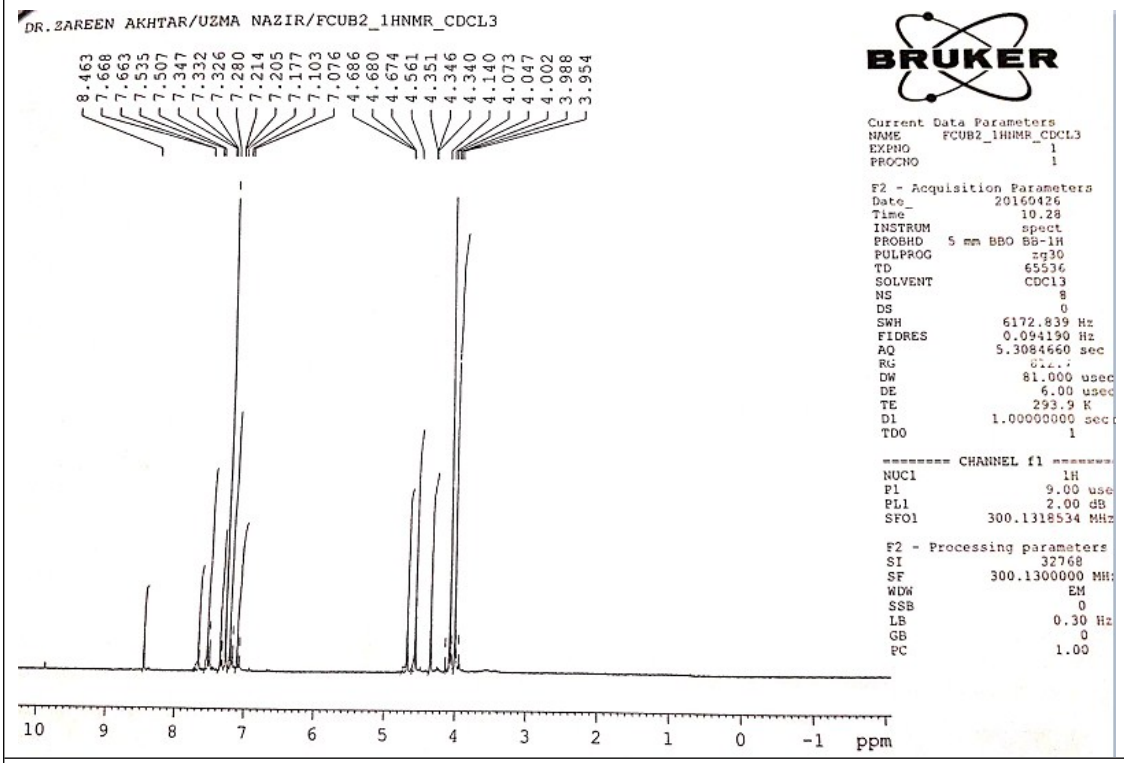

Fig. S4. ^{1}H NMR spectrum of Fcub in $CDCl_3$

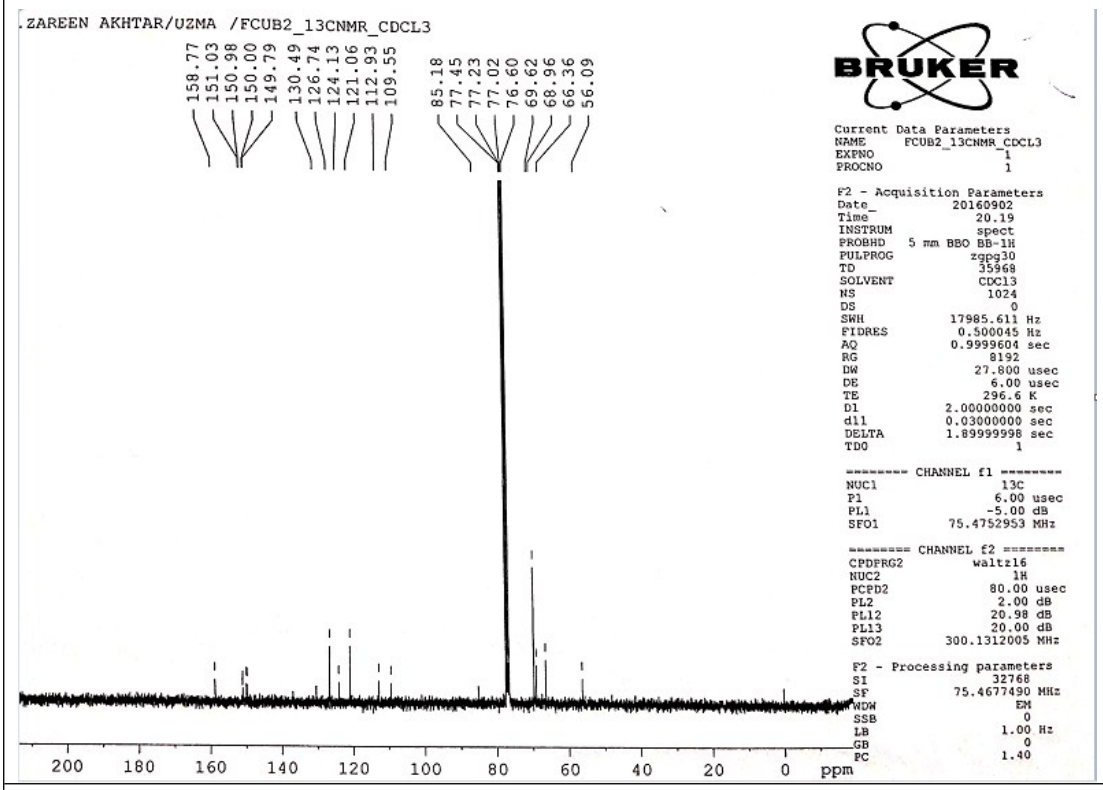

Fig. S5. ^{13}C NMR spectrum of Fcub CDCl3

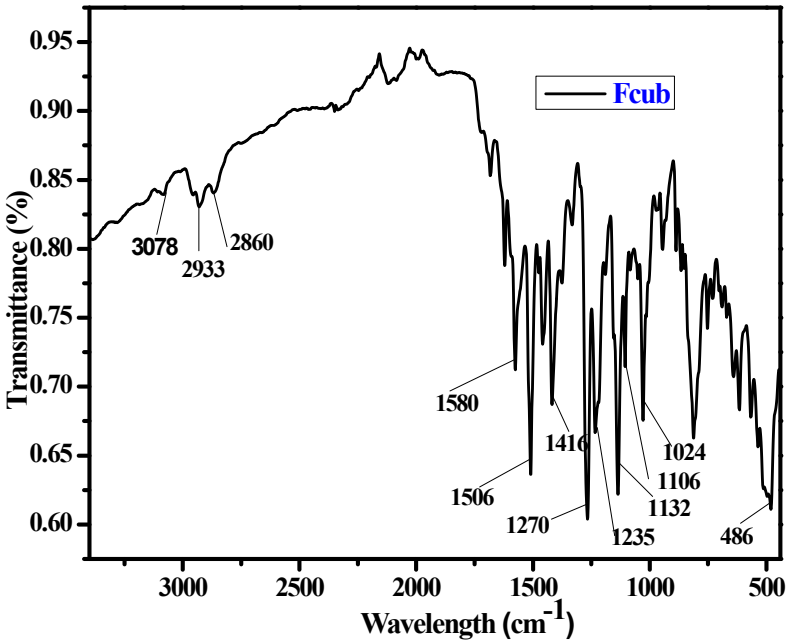

Fig. S6. FT-IR spectrum of Fcub

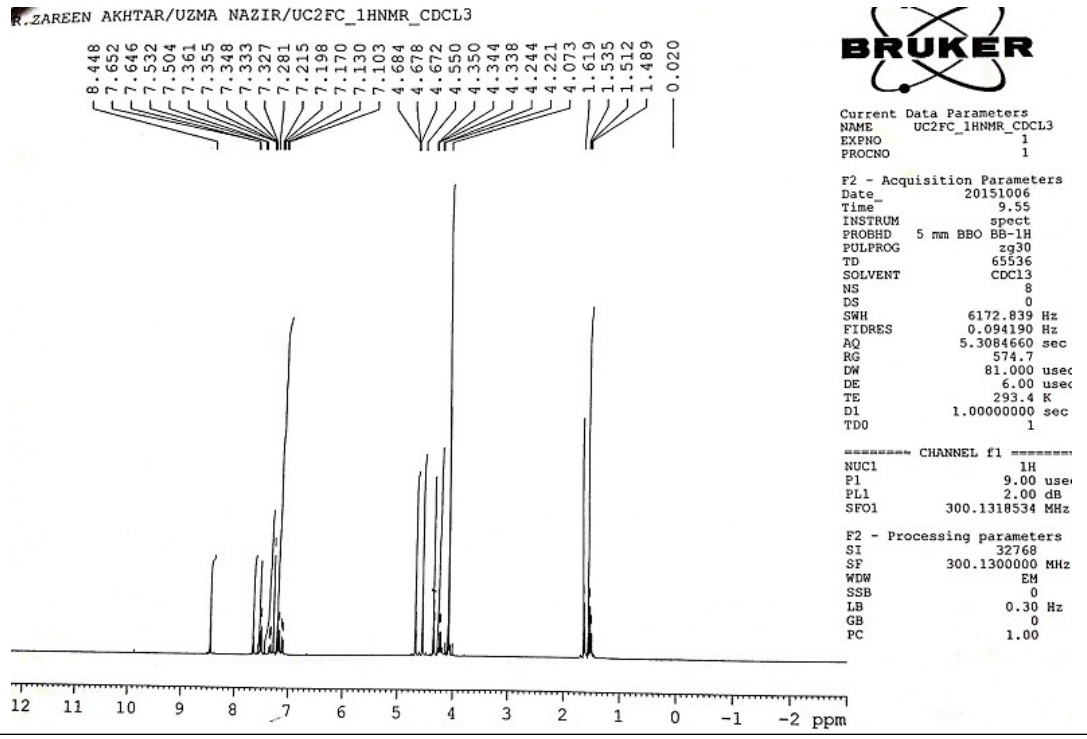

Fig. S7. ^{1}H NMR spectrum of Fcuc in $CDCl_3$

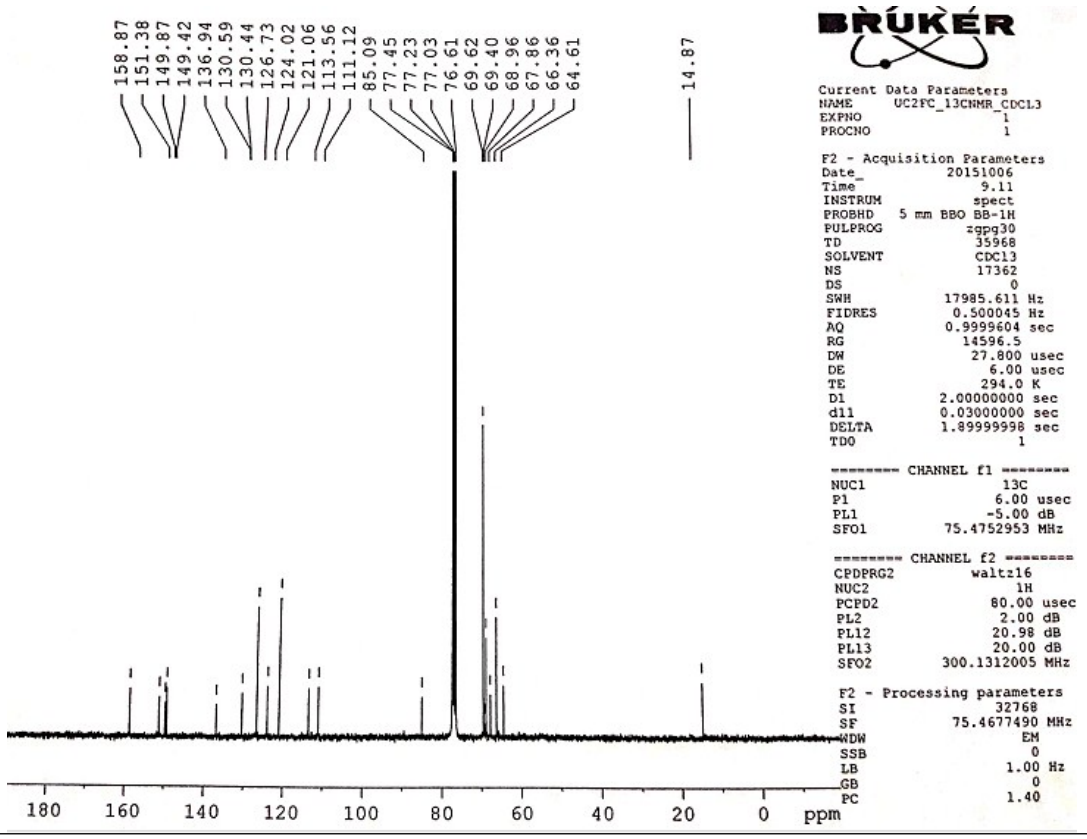

Fig. S8. ^{13}C NMR spectrum of Fcuc in $CDCl_3$

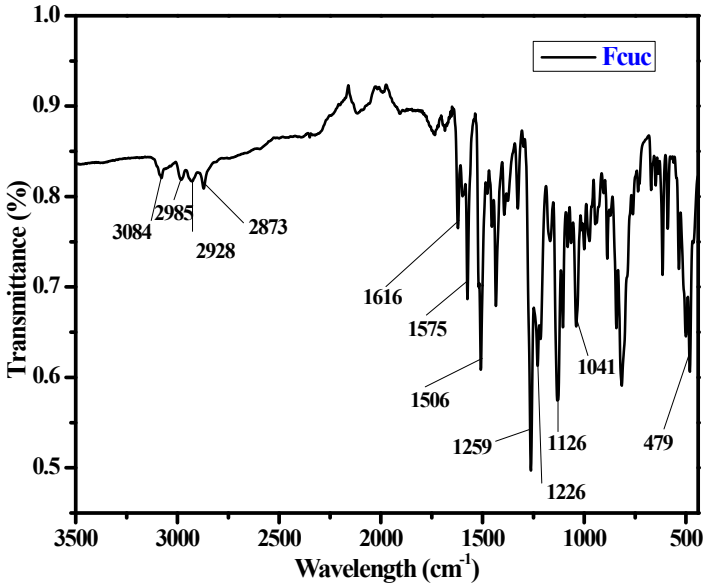

Fig. S9. FT-IR spectrum of Fcuc

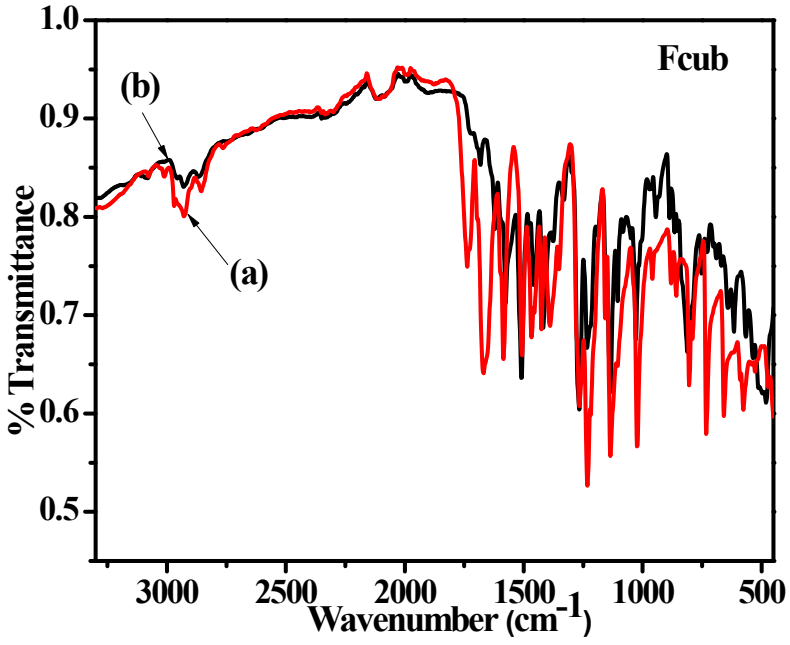

Fig. S10. (a) FT-IR spectra of pure **Fcub** and (b) adsorbed **Fcub** collected from aluminium alloy in 0.1 M HCl.

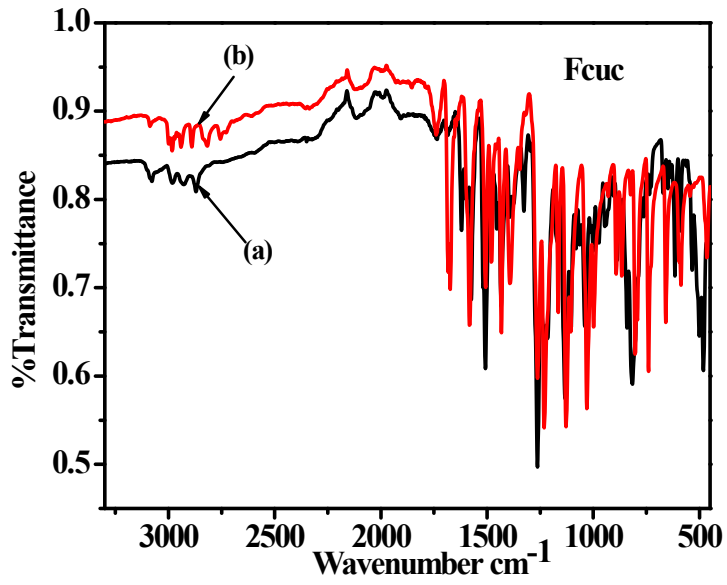

Fig. S11. (a). FT-IR spectra of pure **Fcuc** and (b) adsorbed **Fcuc** collected from aluminium alloy in 0.1 M HCl.

Table S1. FT-IR absorption frequencies of the neat biferrocenyl Schiff base (Fcua) and the corrosion product of inhibited aluminium surface in presence of biferrocenyl Schiff base (Fcua).

Inhibitor before adsorption	Corrosion product of aluminium	Functional group/assignment
3092	3081	C-H aromatic
2870	2875	C-H aliphatic
1602	1592	C=N azomethine
1569	1566	C-C stretches
1372	1367	C-H rocking
1449	1456	C-N stretch
1240	1229	C-O-C stretch
486	480	Fe-Cp

Table S2. Quantum chemical parameters obtained using semi-empirical method with a PM6 basis set for biferrocenyl Schiff bases (Fcua, Fcub, and Fcua).

Quantum Parameters	**Inhibitors**		
	Fcua	**Fcub**	**Fcuc**
E_{HOMO} (eV)	-0.3009	-0.3019	-0.30535
E_{LUMO} (eV)	-0.0231	-0.0265	-0.02465
ΔE (eV)	0.2778	0.2754	0.2807
μ (eV)	3.6	4.8	4.8
I (eV)	0.3009	0.3019	0.30535
A (eV)	0.0231	0.0265	0.02465
χ (eV)	0.1620	0.1640	0.165
η (eV)	0.1380	0.1370	0.136
σ	7.2463	7.2990	7.142
$q_N(83)$	-0.3237	-0.3130	-0.315329
$q_N(84)$	-0.3304	-0.3183	-0.315653
$q_O(85)$	-0.3898	-0.3879	-0.386132
$q_O(86)$	-0.3956	-0.37904	-0.374767
$q_O(87)$	-	-0.38536	-0.426313
$q_O(88)$	-	-0.39153	-0.421965
$q_{Fe}(11)$	0.61	0.60	0.60
$q_{Fe}(73)$	0.43	0.43	0.60

Table S3. Comparison of various ferrocene derivatives as corrosion inhibitors for different metal alloys.

Inhibitors	Conc.	T (K)	Alloys	Medium	Evaluation method Performance (I.E %)	Ref.
4,4'-((((ethane-1,2-diylbis (oxy))bis(4,1-phenylene)) bis(methaneylylidene)) bis(azaneylylidene))bisferrocene **(Fcua)**	100 ppm	298	Aluminium AA2219-T6 alloy	0.1 M HCl	Weight loss (88), EIS (92), Polarization (95.61), FT-IR SEM	This work
4,4'-((((ethane-1,2-diylbis (oxy))bis(2-methoxy-1,4-phenylene)) bis(methaneylylidene)) bis(azaneylylidene))bisferrocene **(Fcub)**	100 ppm	298	Aluminium AA2219-T6 alloy	0.1 M HCl	Weight loss (92), EIS (94), Polarization (98.86), FT-IR, SEM	This work
4,4'-((((ethane-1,2-diylbis (oxy))bis(2-methoxy-1,4-phenylene)) bis(methaneylylidene)) bis(azaneylylidene))bisferrocene **(Fcuc)**	100 ppm	298	Aluminium AA2219-T6 alloy	0.1 M HCl	Weight loss (97), EIS (95), Polarization (99.01), FT-IR, SEM	This work
Ferrocene carboxaldehyde propanoylhydrazone (fcph)	100 ppm	298	Mild steel	0.5 M H_2SO_4	Weight loss (90.7), EIS (86.5), Polarization (90.0)	[6]
Ferrocene carboxaldehyde furoylhydrazone (fcfh)	100 ppm	298	Mild steel	0.5 M H_2SO_4	Weight loss (93.0), EIS (91.1),	[6]

					Polarization (91.2)	
1,1'-diformylferrocene (diformyl Fc)	100 µM	298	Mild steel	0.5 M H_2SO_4	EIS (80), Polarization (82)	[3]
1,1'-diacetylferrocene (Diacetyl Fc)	100 µM	298	Mild steel	0.5 M H_2SO_4	EIS (25), Polarization (32)	[3]
2-benzimidazoylthioacetylferrocene (BIM Fc)	100 µM	298	Mild steel	0.5 M H_2SO_4	EIS (84.2), Polarization (87.7)	[3]