

**Electronic Supplementary Information**

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

**Uzma Nazir<sup>a</sup>, Zareen Akhter<sup>a,\*</sup>, Naveed Kausar Janjua<sup>a</sup>, Muhammad Adeel Asghar<sup>a</sup>, Sehrish Kanwal<sup>a</sup>, Tehmeena Maryum Butt<sup>a</sup>, Asma Sani<sup>a</sup>, Faroha Liaqat<sup>a</sup>, Rizwan Hussain<sup>b</sup> and Faiz Ullah Shah<sup>c,\*</sup>**

<sup>a</sup>*Department of Chemistry, Quaid-i-Azam University, Islamabad-45320, Pakistan*

<sup>b</sup>*National Center for Physics, Quaid-i-Azam University Campus, Islamabad, Pakistan.*

<sup>c</sup>*Chemistry of Interfaces, Luleå University of Technology, 971 87 Luleå, Sweden*

\*Corresponding author's mail: [zareen\\_a@qau.edu.pk](mailto:zareen_a@qau.edu.pk) and [faiz.ullah@ltu.se](mailto:faiz.ullah@ltu.se)

DR.ZAREEN AKHTAR/UZMA NAZIR/FCUA2\_1HNMR\_CDCl<sub>3</sub>



Current Data Parameters  
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EXPNO 1  
PROCNO 1

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NS 8  
DS 0  
SWH 6172.839 Hz  
FIDRES 0.094190 Hz  
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RG 12.1  
DW 81.000 usec  
DE 6.00 usec  
TE 294.0 K  
D1 1.0000000 sec  
TDO 1

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PL1 2.00 dB  
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F2 - Processing parameters  
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SF 300.1300000 MHz\*  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm

Fig. S1. <sup>1</sup>H NMR spectrum of Fcua in CDCl<sub>3</sub>



Current Data Parameters  
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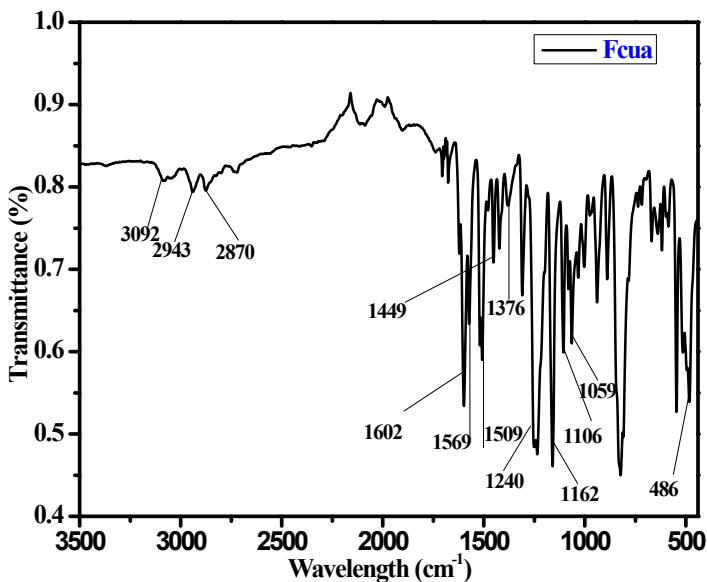
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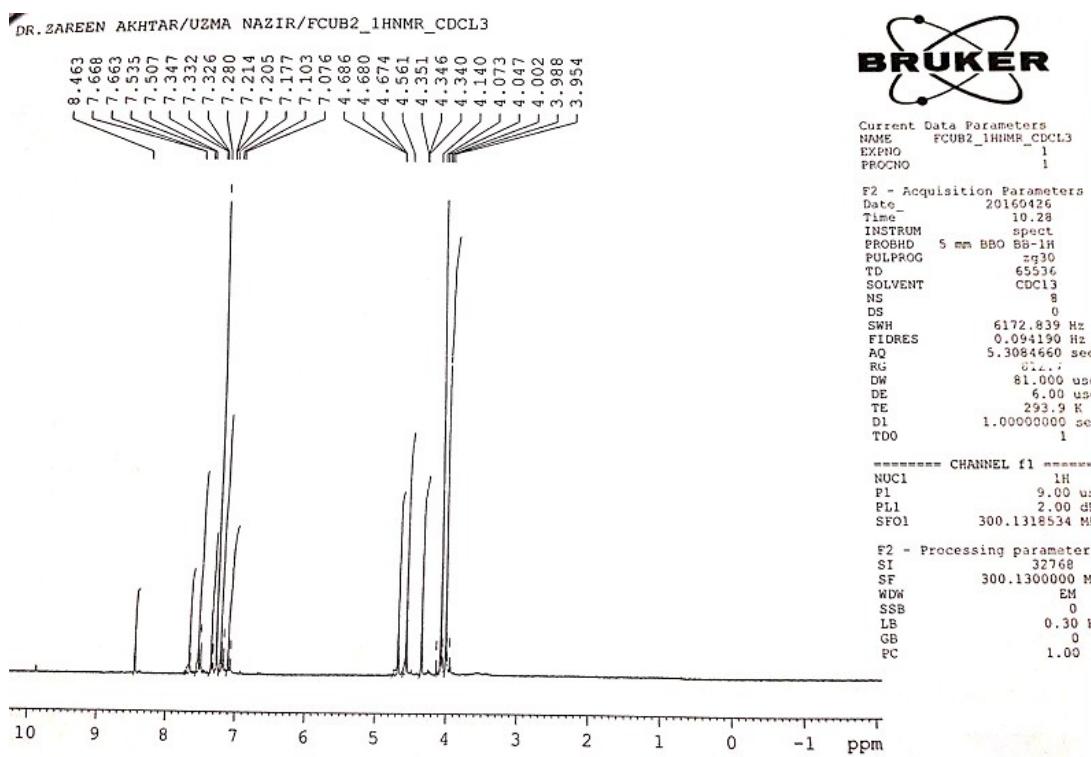
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Fig. S2. <sup>13</sup>C NMR spectrum of Fcua CDCl<sub>3</sub>



**Fig. S3.** FT-IR spectrum of Fcua



**Fig. S4.**  $^1\text{H}$  NMR spectrum of Fcub in  $\text{CDCl}_3$

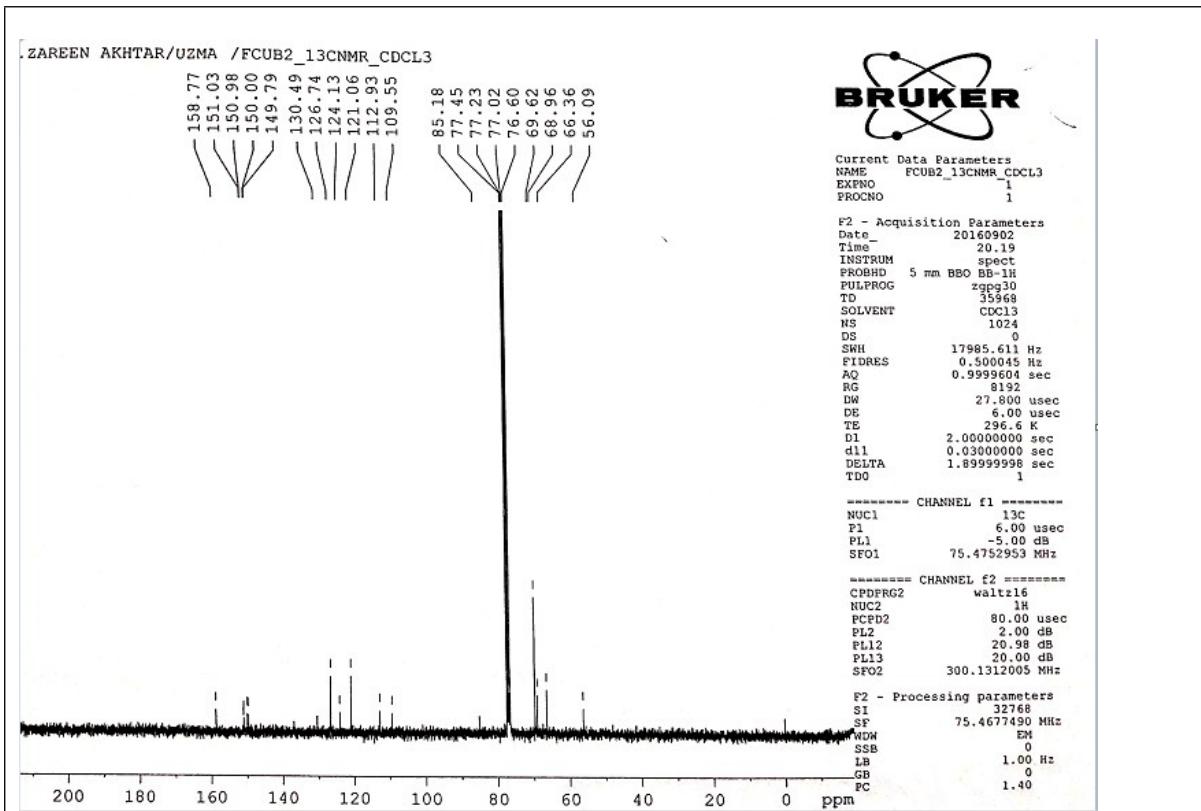


Fig. S5.  $^{13}\text{C}$  NMR spectrum of Fcub CDCl3

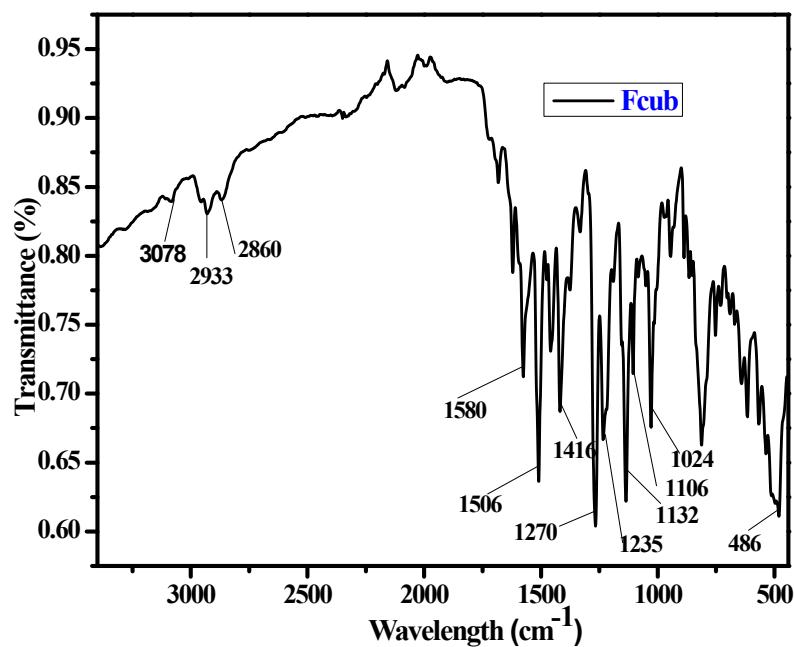


Fig. S6. FT-IR spectrum of Fcub

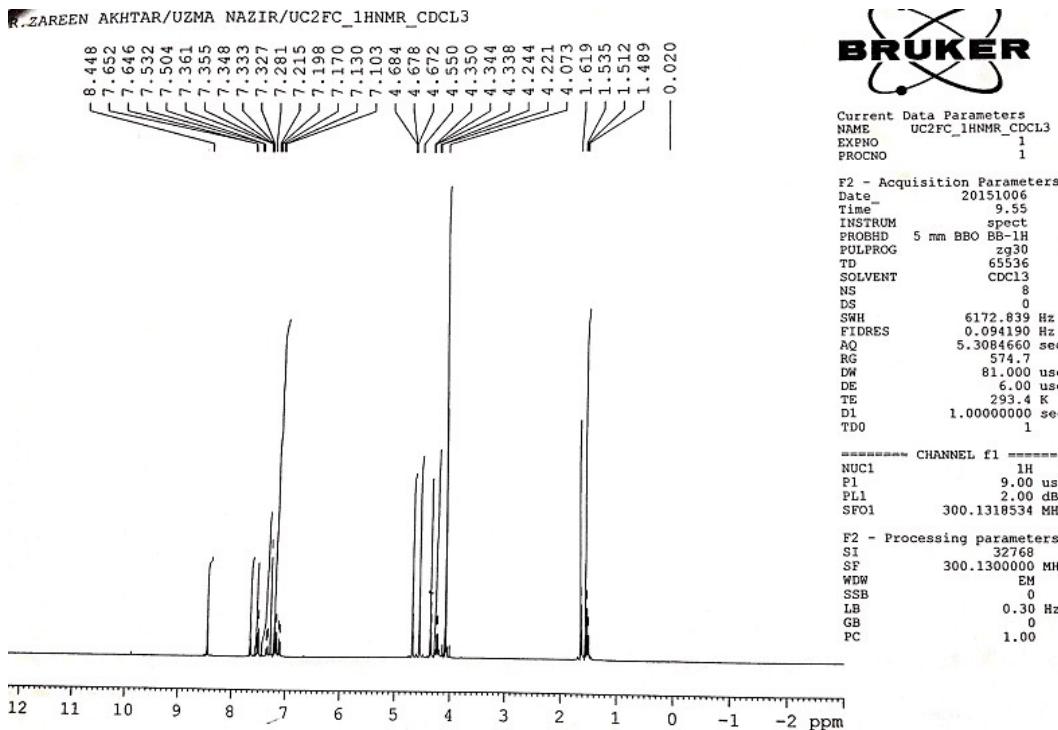


Fig. S7.  $^1\text{H}$  NMR spectrum of Fcuc in  $\text{CDCl}_3$

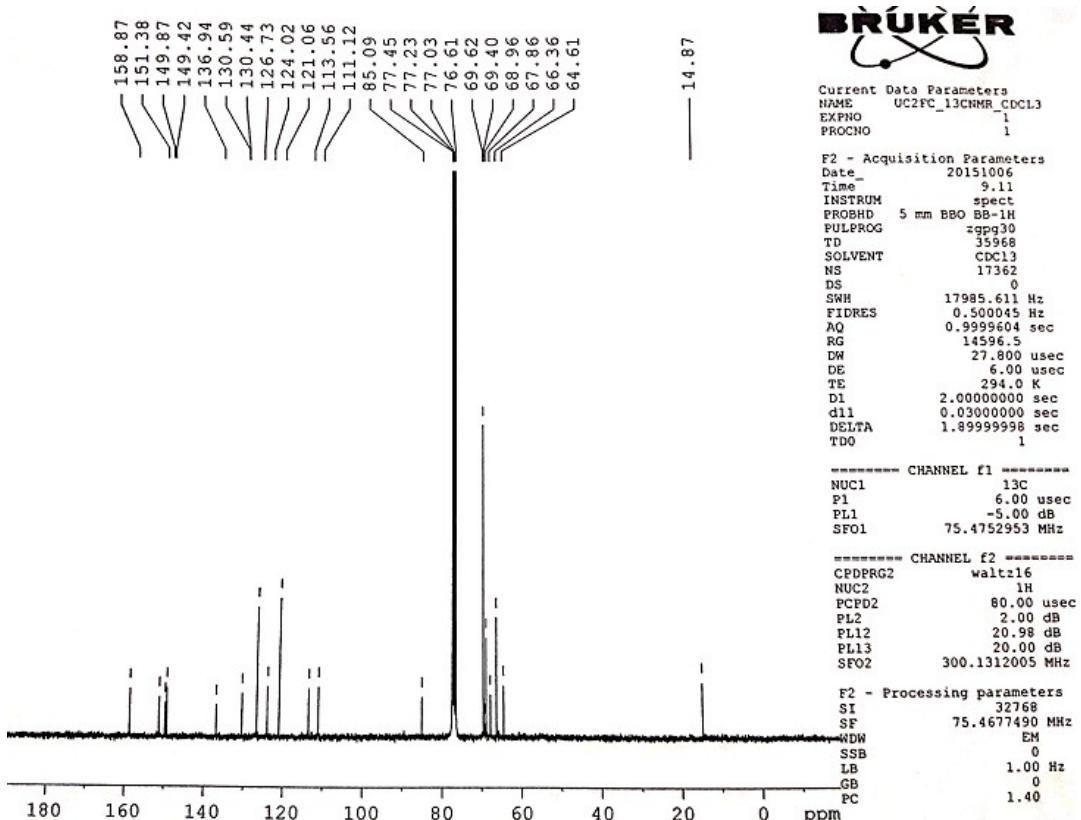
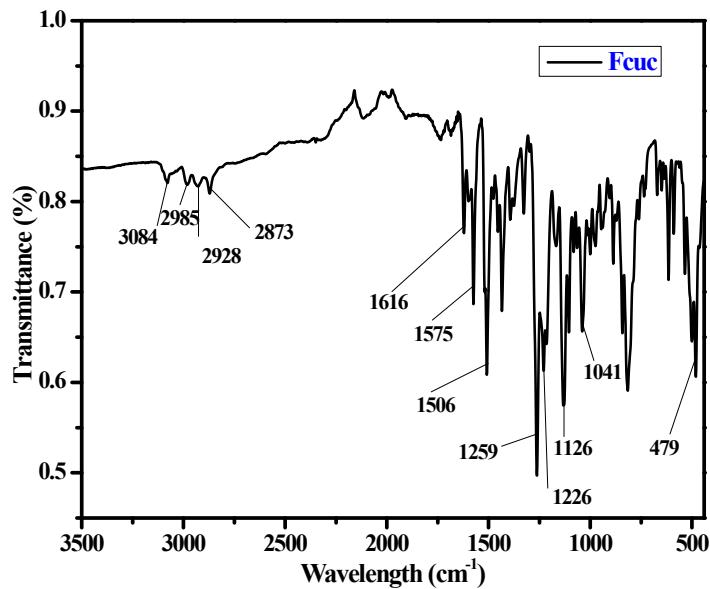
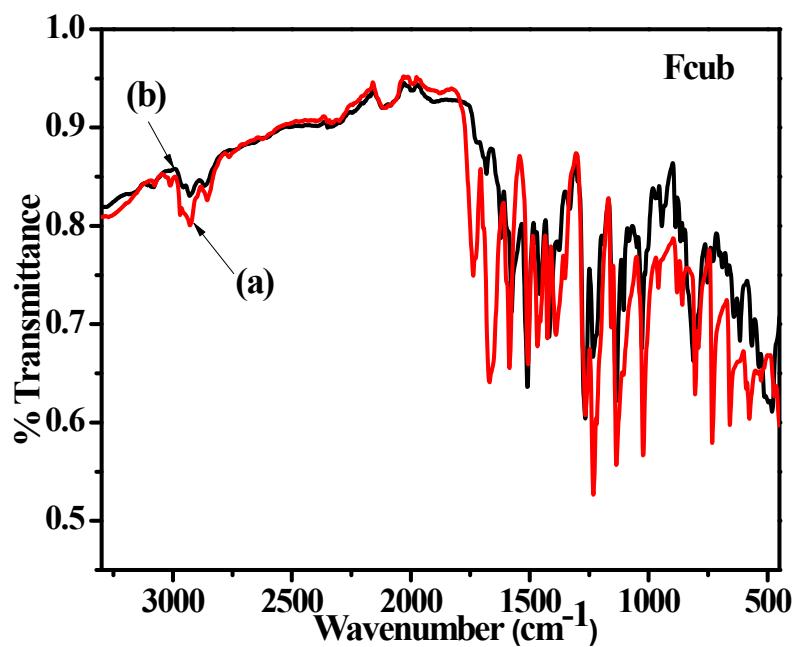


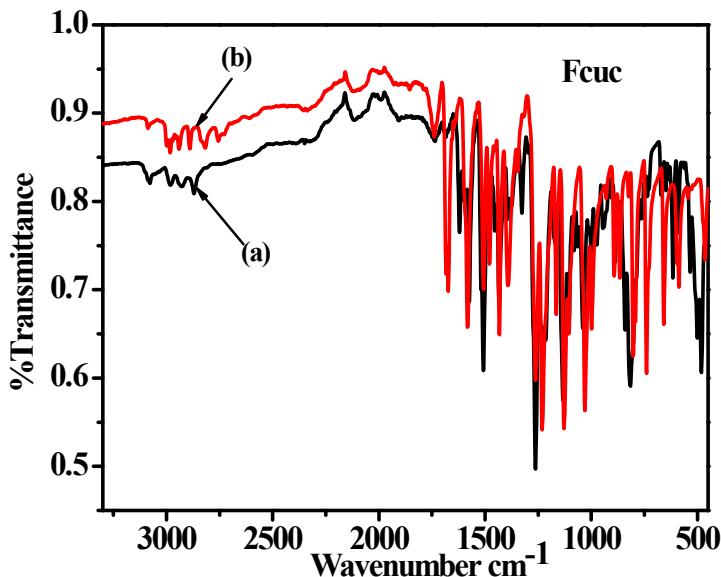
Fig. S8.  $^{13}\text{C}$  NMR spectrum of Fcuc in  $\text{CDCl}_3$



**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 Fcuc).

Quantum Parameters	Inhibitors		
	Fcua	Fcub	Fcuc
E <sub>HOMO</sub> (eV)	-0.3009	-0.3019	-0.30535
E <sub>LUMO</sub> (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 <sub>N</sub> (83)	-0.3237	-0.3130	-0.315329
q <sub>N</sub> (84)	-0.3304	-0.3183	-0.315653
q <sub>O</sub> (85)	-0.3898	-0.3879	-0.386132
q <sub>O</sub> (86)	-0.3956	-0.37904	-0.374767
q <sub>O</sub> (87)	-	-0.38536	-0.426313
q <sub>O</sub> (88)	-	-0.39153	-0.421965
q <sub>Fe</sub> (11)	0.61	0.60	0.60
q <sub>Fe</sub> (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 <sub>2</sub> SO <sub>4</sub>	Weight loss (90.7), EIS (86.5), Polarization (90.0)	[6]
Ferrocene carboxaldehyde furoylhydrazone (fcfh)	100 ppm	298	Mild steel	0.5 M H <sub>2</sub> SO <sub>4</sub>	Weight loss (93.0), EIS (91.1),	[6]

				Polarization (91.2)	
1,1'-diformylferrocene (diformyl Fc)	100 $\mu\text{M}$	298	Mild steel	0.5 M $\text{H}_2\text{SO}_4$ EIS (80), Polarization (82)	[3]
1,1'-diacetylferrocene (Diacetyl Fc)	100 $\mu\text{M}$	298	Mild steel	0.5 M $\text{H}_2\text{SO}_4$ EIS (25), Polarization (32)	[3]
2-benzimidazoylthioacetylferrocene (BIM Fc)	100 $\mu\text{M}$	298	Mild steel	0.5 M $\text{H}_2\text{SO}_4$ EIS (84.2), Polarization (87.7)	[3]