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Experimental and Theoretical Investigations of Michelia Alba Leaves Extract as a Green Highly-effective Corrosion Inhibitor for Different Steel Materials in Acidic Solution

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Fig. S1 Michelia alba leaves

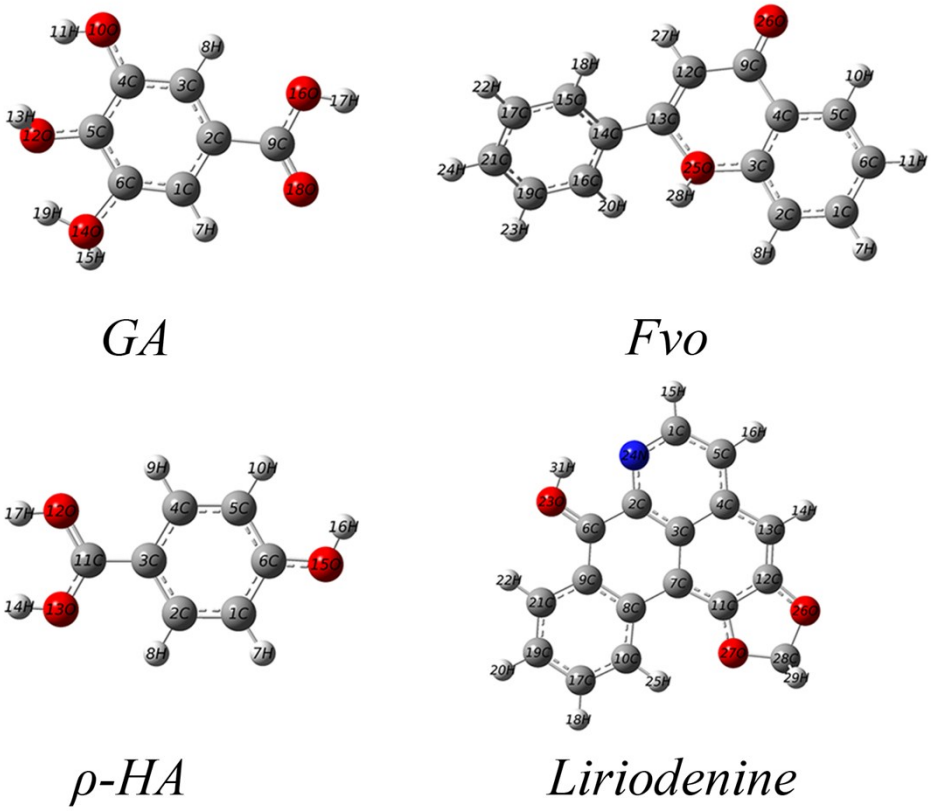

Fig. S2 Optimized structures of molecules of the major effective components of MALE in the protonated form.

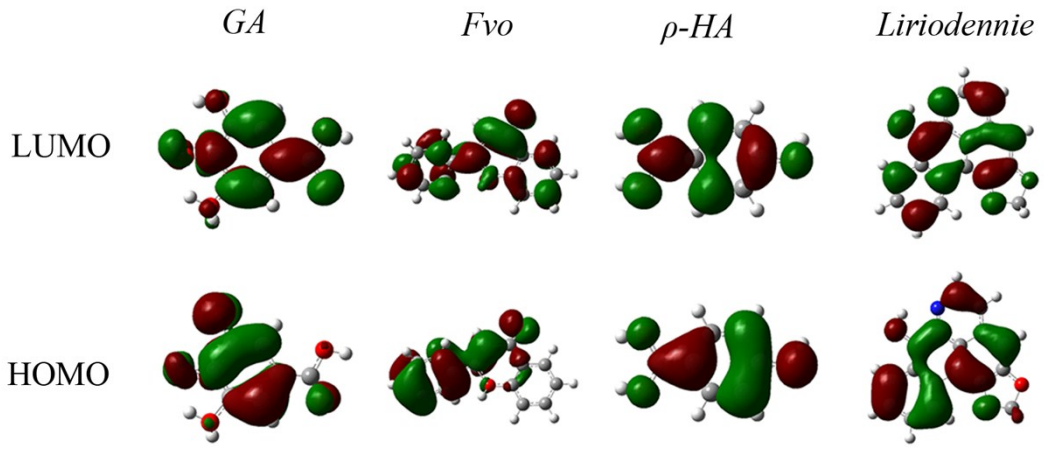

Fig. S3 LUMO and HOMO distribution of the calculated molecules in the protonated form.

Table S1 Chemical compositions of three steel materials used in the present work

Steel materials	Chemical compositions (wt.%)						
	C	Mn	Si	P	S	Cr	Fe
Industrial-pure iron	0.04	0.30	0.20	0.03	0.02	-	Bal.
303 stainless steel	0.10	1.50	0.05	0.20	0.15	17	Bal.
Q235 carbon steel	0.17	0.46	0.26	0.0047	0.017	-	Bal.

Table S2 Identification of FTIR bands of different samples in Fig. 5 to corresponding functional groups

	MALE powder	Industrial -pure iron	303 stainless steel	Q235 carbon steel
O—H stretching vibration[1,2]	3425.28	3438.92	3445.32	3448.15
C—H asymmetrical stretching vibration[1,3]	2925.18	2917.59	2924.46	2922.85
C—H symmetric stretching vibration[1]	2854.64	2855.85	2853.78	2852.29
C==O stretching vibrations[2]	1626.78	1644.71	1633.49	1637.38
C==C stretching vibrations[4]	1538.96	1538.36	1567.58	1566.13
C==C stretching vibrations[5]	1417.18	1454.60	1462.85	1462.27
symmetrical ring breathing vibration of the epoxy group[6]	1264.36	—	1280.26	1280.15
framework vibration of aromatic ring[1]	1116.90	1109.68	1117.84	1146.29
C—O—C asymmetric stretching vibration[2]	1073.96	—	—	1087.40
C—N stretching vibration[1]	1048.77	1029.18	—	—
C—H out of plane bending vibration of the aromatic ring[6]	894.71	890.92	947.31	761.29
C==C out of plane bending vibration of the aromatic ring[6]	601.55	666.35	—	599.70

Table S3 Calculated quantum chemical parameters for the major effective components of MALE in the protonated form.

	GA	Fvo	ρ-HA	Liriodenine
E_{HOMO} (eV)	-10.84	-10.64	-10.87	-9.91
E_{LUMO} (eV)	-5.42	-6.13	-6.69	-6.98
ΔE (eV)	5.42	4.51	4.18	2.93
μ(D)	8.96	5.48	5.51	1.37
$\langle\alpha\rangle$	85.20	163.45	87.01	212.85
η (eV)	2.71	2.26	2.09	1.46
σ (eV^{-1})	0.37	0.44	0.48	0.68
Pi (eV)	-8.13	-8.38	-8.78	-8.44
χ (eV)	8.13	8.38	8.78	8.44
ω	12.20	15.54	18.44	24.42

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