Experimental and theoretical investigations into green approach steel corrosion inhibition performance of aqueous mixture of *Olea europaea* and *Ficus carica* leaves extract in acid medium

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2.1. Extraction of *Olea europaea and Ficus carica leaves*

Olea europaea and *Ficus carica* leaves leaves were harvested in a farm located around Guelma, Algeria. Leaves were separated from the stalk and rinsed thoroughly with tap water and left away to dry in a well-ventilated area shielded from sunlight. Three weeks later, the dry leaves were pulverized into a fine powder, using an electric grinder. Then, an equimass mixture-of *Olea europaea* and *Ficus carica* leaves powder and distilled water was (50 g/500mL) was put under stirring at 40 °C for 3 hours. After 30 minutes of ultrasonic treatment, the mixture was filtered. Finally, in order to use the recovered filtrate as a green inhibitor, it was put in a vial and kept in the refrigerator.

2.2. Preparation of steel samples

Corrosion tests were conducted on Mild steel (MS). Mild steel plate was cut into rectangular specimen (surface area of 1×2 cm^2). The metal pieces were mechanically polished to a mirror-like finish. Finally, after a double cleaning with distilled water and ethanol, samples were dried and stored till use.

2.3. Preparation of the solution

1 M HCl, the corrosive solution, was prepared by using a 37% concentrated commercial hydrochloric acid solution. FLE was incorporated into the corrosive solution with different amounts 0.05-0.25 V/V.

Table S1: Inhibitory efficiency as a function of OFLE concentrations at various temperatures

	EI%				
T (K)	**298**	**308**	**318**	**328**	**338**
C (ml/ml)					
0.00	-	-	-	-	-
0.05	67.47	63.76	72.34	82.16	90.56
0.10	79.91	77.59	79.41	86.01	94.26
0.15	65.55	68.89	74.87	85.94	94.27
0.20	78.43	65.67	75.71	85.76	94.74
0.25	80.02	81.01	84.95	89.68	95.19

Table S2: Electrophilic $f_k^-(r)$. Nucleophilic $f_k^+(r)$ Condensed Fukui Functions and Condensed Dual Descriptor Δf_k (r) over the Atoms of the Psoralen. Bergapten. Hydroxytyrosol. Luteolin-7-O-glucoside and Oleuropein.

		Psoralen					
Position	Atom	N	N+1	N-1	$f_k^+(r)$	$f_k^-(r)$	$\Delta f_k(r)$
1	O	-0.5082	-0.45097	-0.54425	0.05723	0.03605	0.04664
2	C	0.75853	0.74638	0.71374	-0.01215	0.04479	0.01632
3	O	-0.56865	-0.42753	-0.68578	0.14112	0.11713	0.129125
4	C	-0.34139	-0.26241	-0.4569	0.07898	0.11551	0.097245
5	C	-0.15065	-0.15273	-0.28745	-0.00208	0.1368	0.06736
6	C	-0.15641	-0.10708	-0.14513	0.04933	-0.01128	0.019025
7	C	-0.16454	-0.14491	-0.28556	0.01963	0.12102	0.070325
8	C	-0.13208	-0.05413	-0.13844	0.07795	0.00636	0.042155
9	C	-0.31652	-0.26775	-0.34195	0.04877	0.02543	0.0371
10	C	0.11704	0.25618	0.0426	0.13914	0.07444	0.10679
11	O	-0.46636	-0.44512	-0.48738	0.02124	0.02102	0.02113
12	C	0.33135	0.37719	0.28087	0.04584	0.05048	0.04816
13	C	-0.29506	-0.26469	-0.3668	0.03037	0.07174	0.051055
14	C	0.34715	0.44982	0.35055	0.10267	-0.0034	0.049635
15	H	0.26778	0.29891	0.2299	0.03113	0.03788	0.034505
16	H	0.25122	0.28154	0.21219	0.03032	0.03903	0.034675
17	H	0.2469	0.28115	0.21492	0.03425	0.03198	0.033115
18	H	0.26189	0.29741	0.23597	0.03552	0.02592	0.03072
19	H	0.24224	0.27869	0.21215	0.03645	0.03009	0.03327
20	H	0.27574	0.31006	0.24675	0.03432	0.02899	0.031655

		Bergapten					
Position	Atom	N	N+1	N-1	$f_k^+(r)$	$f_k^-(r)$	$\Delta f_k(r)$
1	O	-0.5532	-0.45449	-0.57386	0.09871	0.02066	0.059685
2	C	-0.3247	-0.34488	-0.3135	-0.02018	-0.0112	-0.01569
3	C	0.45217	0.55353	0.34166	0.10136	0.11051	0.105935
4	C	-0.2176	-0.18062	-0.1947	0.03698	-0.0229	0.00704
5	C	-0.21253	-0.1851	-0.21139	0.02743	-0.00114	0.013145
6	C	0.36364	0.37325	0.35739	0.00961	0.00625	0.00793
7	C	-0.1488	-0.16983	-0.30975	-0.02103	0.16095	0.06996
8	C	0.34239	0.31217	0.28983	-0.03022	0.05256	0.01117
9	C	-0.32713	-0.2537	-0.35452	0.07343	0.02739	0.05041
10	C	-0.32589	-0.16188	-0.37844	0.16401	0.05255	0.10828
11	O	-0.50931	-0.47366	-0.54794	0.03565	0.03863	0.03714
12	C	-0.35012	-0.25815	-0.46347	0.09197	0.11335	0.10266
13	O	-0.46484	-0.40004	-0.48579	0.0648	0.02095	0.042875
14	C	0.11161	0.19976	0.04535	0.08815	0.06626	0.077205
15	C	0.75839	0.74405	0.71148	-0.01434	0.04691	0.016285
16	O	-0.57277	-0.49625	-0.68921	0.07652	0.11644	0.09648
17	H	0.24197	0.27353	0.21948	0.03156	0.02249	0.027025
18	H	0.21551	0.23699	0.20051	0.02148	0.015	0.01824
19	H	0.21552	0.237	0.20052	0.02148	0.015	0.01824
20	H	0.26584	0.28458	0.23156	0.01874	0.03428	0.02651
21	H	0.25667	0.28526	0.23451	0.02859	0.02216	0.025375
22	H	0.27523	0.30744	0.24795	0.03221	0.02728	0.029745
23	H	0.26573	0.29383	0.22847	0.0281	0.03726	0.03268
24	H	0.24221	0.27721	0.21385	0.035	0.02836	0.03168

		Hydroxytyrosol					
Position	Atom	N	N+1	N-1	$f_k^+(r)$	$f_k^-(r)$	$\Delta f_k(r)$
1	C	0.38412	0.38003	0.70128	-0.00409	-0.31716	-0.160625
2	N	-0.94254	-0.90086	-0.45839	0.04168	-0.48415	-0.221235
3	C	-0.11603	-0.11121	-0.28808	0.00482	0.17205	0.088435
4	C	-0.48711	-0.51687	-0.11299	-0.02976	-0.37412	-0.20194
5	C	-0.07524	0.10235	-0.26293	0.17759	0.18769	0.18264
6	C	-0.2137	-0.19392	0.25408	0.01978	-0.46778	-0.224
7	C	-0.27672	-0.21913	-0.56878	0.05759	0.29206	0.174825
8	C	0.30475	0.40157	-0.31077	0.09682	0.61552	0.35617
9	O	-0.708	-0.58036	0.16265	0.12764	-0.87065	-0.371505
10	C	-0.31191	-0.24102	-0.75226	0.07089	0.44035	0.25562
11	C	-0.22699	-0.20317	-0.30618	0.02382	0.07919	0.051505
12	O	-0.79551	-0.72354	-0.27626	0.07197	-0.51925	-0.22364
13	O	-0.77225	-0.7593	-0.73191	0.01295	-0.04034	-0.013695
14	H	0.18174	0.21109	-0.7738	0.02935	0.95554	0.492445
15	H	0.40208	0.39603	0.2191	-0.00605	0.18298	0.088465
16	H	0.40065	0.41786	0.22363	0.01721	0.17702	0.097115
17	H	0.23444	0.25617	0.23042	0.02173	0.00402	0.012875
18	H	0.24621	0.27154	0.20938	0.02533	0.03683	0.03108
19	H	0.27469	0.3097	0.21028	0.03501	0.06441	0.04971
20	H	0.24592	0.28142	0.21028	0.0355	0.03564	0.03557
21	H	0.25544	0.29324	0.49351	0.0378	-0.23807	-0.100135
22	H	0.50319	0.53247	0.2089	0.02928	0.29429	0.161785
23	H	0.23634	0.27481	0.22983	0.03847	0.00651	0.02249
24	H	0.24402	0.28012	0.48899	0.0361	-0.24497	-0.104435
25	H	0.50653	0.51628	0.47202	0.00975	0.03451	0.02213
26	H	0.50588	0.52469	0.46626	0.01881	0.03962	0.029215

		Luteolin-7-O-glucoside					
Position	Atom	N	N+1	N-1	$f_k^+(r)$	$f_k^-(r)$	$\Delta f_k(r)$
1	C	0.36152	0.36742	0.28992	0.0059	0.0716	0.03875
2	C	-0.3506	-0.21731	-0.39584	0.13329	0.04524	0.089265
3	C	0.4824	0.45935	0.42622	-0.02305	0.05618	0.016565
4	O	-0.57895	-0.51218	-0.66369	0.06677	0.08474	0.075755
5	C	-0.23639	-0.21891	-0.22296	0.01748	-0.01343	0.002025
6	C	0.37528	0.41204	0.34526	0.03676	0.03002	0.03339
7	O	-0.66357	-0.60951	-0.67467	0.05406	0.0111	0.03258
8	C	-0.35359	-0.31262	-0.37432	0.04097	0.02073	0.03085
9	C	0.355	0.36717	0.33141	0.01217	0.02359	0.01788
10	C	-0.36922	-0.2629	-0.3869	0.10632	0.01768	0.062
11	C	0.36439	0.35048	0.36836	-0.01391	-0.00397	-0.00894
12	O	-0.4891	-0.45409	-0.50594	0.03501	0.01684	0.025925
13	C	-0.10319	-0.07865	-0.12041	0.02454	0.01722	0.02088
14	C	-0.23607	-0.23414	-0.28537	0.00193	0.0493	0.025615
15	C	0.27109	0.30713	0.26502	0.03604	0.00607	0.021055
16	O	-0.71172	-0.6659	-0.72894	0.04582	0.01722	0.03152
17	C	0.25221	0.31692	0.18177	0.06471	0.07044	0.067575
18	O	-0.73139	-0.68366	-0.7564	0.04773	0.02501	0.03637
19	C	-0.29971	-0.29442	-0.31714	0.00529	0.01743	0.01136
20	C	-0.20286	-0.15141	-0.238	0.05145	0.03514	0.043295
21	O	-0.52844	-0.50128	-0.53973	0.02716	0.01129	0.019225
22	C	0.37355	0.36977	0.37331	-0.00378	0.00024	-0.00177
23	C	0.0318	0.0304	0.03096	-0.0014	0.00084	-0.00028
24	O	-0.76651	-0.75177	-0.7746	0.01474	0.00809	0.011415
25	C	0.03396	0.03258	-0.04931	-0.00138	0.08327	0.040945
26	O	-0.78258	-0.78543	-0.79786	-0.00285	0.01528	0.006215
27	C	0.03397	0.03202	-0.00693	-0.00195	0.0409	0.019475
28	O	-0.78196	-0.77716	-0.78699	0.0048	0.00503	0.004915
29	C	0.02837	0.026	0.02851	-0.00237	-0.00014	-0.001255

30	O	-0.60479	-0.60147	-0.60623	0.00332	0.00144	0.00238
31	C	-0.14093	-0.14452	-0.14714	-0.00359	0.00621	0.00131
32	O	-0.77635	-0.78401	-0.77437	-0.00766	-0.00198	-0.00482
33	H	0.25589	0.27512	0.23793	0.01923	0.01796	0.018595
34	H	0.5011	0.52035	0.48722	0.01925	0.01388	0.016565
35	H	0.24853	0.27271	0.2315	0.02418	0.01703	0.020605
36	H	0.28156	0.2984	0.27413	0.01684	0.00743	0.012135
37	H	0.26435	0.27727	0.25193	0.01292	0.01242	0.01267
38	H	0.52282	0.5344	0.51292	0.01158	0.0099	0.01074
39	H	0.518	0.53499	0.5048	0.01699	0.0132	0.015095
40	H	0.24253	0.26752	0.22087	0.02499	0.02166	0.023325
41	H	0.24787	0.26177	0.23514	0.0139	0.01273	0.013315
42	H	0.21445	0.21564	0.21421	0.00119	0.00024	0.000715
43	H	0.25661	0.26329	0.24985	0.00668	0.00676	0.00672
44	H	0.51545	0.51882	0.5144	0.00337	0.00105	0.00221
45	H	0.24693	0.25915	0.23063	0.01222	0.0163	0.01426
46	H	0.50602	0.51367	0.46588	0.00765	0.04014	0.023895
47	H	0.22286	0.2332	0.20951	0.01034	0.01335	0.011845
48	H	0.50527	0.50892	0.49942	0.00365	0.00585	0.00475
49	H	0.25312	0.26052	0.24363	0.0074	0.00949	0.008445
50	H	0.22775	0.22803	0.22802	0.00028	-0.00027	5E-06
51	H	0.20949	0.22245	0.19792	0.01296	0.01157	0.012265
52	H	0.5038	0.50384	0.50312	0.00004	0.00068	0.00036

		Oleuropein					
Position	Atom	N	N+1	N-1	$f_k^+(r)$	$f_k^-(r)$	$\Delta f_k(r)$
1	C	0.27682	0.36742	0.26	0.0906	0.01682	0.05371
2	C	0.26693	-0.21731	0.2324	-0.48424	0.03453	-0.224855
3	C	-0.29332	0.45935	-0.31391	0.75267	0.02059	0.38663
4	C	-0.05488	-0.51218	-0.0582	-0.4573	0.00332	-0.22699
5	C	-0.24383	-0.21891	-0.24815	0.02492	0.00432	0.01462
6	C	-0.29565	0.41204	-0.34582	0.70769	0.05017	0.37893
7	O	-0.69499	-0.60951	-0.71309	0.08548	0.0181	0.05179
8	O	-0.69403	-0.31262	-0.70308	0.38141	0.00905	0.19523
9	C	-0.49626	0.36717	-0.49855	0.86343	0.00229	0.43286
10	C	-0.11737	-0.2629	-0.11713	-0.14553	-0.00024	-0.072885
11	O	-0.56952	0.35048	-0.5718	0.92	0.00228	0.46114
12	C	0.83618	-0.45409	0.83686	-1.29027	-0.00068	-0.645475
13	C	-0.54452	-0.07865	-0.54354	0.46587	-0.00098	0.232445
14	O	-0.6094	-0.23414	-0.61769	0.37526	0.00829	0.191775
15	C	-0.29317	0.30713	-0.29087	0.6003	-0.0023	0.299
16	C	-0.09778	-0.6659	-0.08081	-0.56812	-0.01697	-0.292545
17	C	0.38699	0.31692	0.38638	-0.07007	0.00061	-0.03473
18	O	-0.54829	-0.68366	-0.55876	-0.13537	0.01047	-0.06245
19	C	0.21907	-0.29442	0.14656	-0.51349	0.07251	-0.22049
20	C	-0.25029	-0.15141	-0.26966	0.09888	0.01937	0.059125
21	C	0.79496	-0.50128	0.75072	-1.29624	0.04424	-0.626
22	O	-0.62434	0.36977	-0.67246	0.99411	0.04812	0.521115
23	O	-0.57449	0.0304	-0.58683	0.60489	0.01234	0.308615
24	C	-0.33328	-0.75177	-0.3289	-0.41849	-0.00438	-0.211435
25	C	-0.16273	0.03258	-0.18277	0.19531	0.02004	0.107675
26	C	-0.72631	-0.78543	-0.72155	-0.05912	-0.00476	-0.03194
27	O	-0.57182	0.03202	-0.5781	0.60384	0.00628	0.30506
28	C	0.38693	-0.77716	0.38649	-1.16409	0.00044	-0.581825
29	C	0.00699	0.026	-0.00103	0.01901	0.00802	0.013515

30	O	-0.77893	-0.60147	-0.78589	0.17746	0.00696	0.09221
31	C	0.03827	-0.14452	-0.09528	-0.18279	0.13355	-0.02462
32	O	-0.78021	-0.78401	-0.81061	-0.0038	0.0304	0.0133
33	C	0.03437	0.27512	-0.06503	0.24075	0.0994	0.170075
34	O	-0.78411	0.52035	-0.78883	1.30446	0.00472	0.65459
35	C	0.02878	0.27271	0.027	0.24393	0.00178	0.122855
36	O	-0.5898	0.2984	-0.59744	0.8882	0.00764	0.44792
37	C	-0.13517	0.27727	-0.1732	0.41244	0.03803	0.225235
38	O	-0.77667	0.5344	-0.78331	1.31107	0.00664	0.658855
39	H	0.2325	0.53499	0.22826	0.30249	0.00424	0.153365
40	H	0.24357	0.26752	0.23834	0.02395	0.00523	0.01459
41	H	0.23685	0.26177	0.22506	0.02492	0.01179	0.018355
42	H	0.50211	0.21564	0.46699	-0.28647	0.03512	-0.125675
43	H	0.50215	0.26329	0.48525	-0.23886	0.0169	-0.11098
44	H	0.25217	0.51882	0.24973	0.26665	0.00244	0.134545
45	H	0.25685	0.25915	0.25353	0.0023	0.00332	0.00281
46	H	0.23791	0.51367	0.23525	0.27576	0.00266	0.13921
47	H	0.23281	0.2332	0.23031	0.00039	0.0025	0.001445
48	H	0.26974	0.50892	0.2671	0.23918	0.00264	0.12091
49	H	0.27769	0.26052	0.27921	-0.01717	-0.00152	-0.009345
50	H	0.29871	0.22803	0.29114	-0.07068	0.00757	-0.031555
51	H	0.22151	0.22245	0.21769	0.00094	0.00382	0.00238
52	H	0.24567	0.50384	0.23472	0.25817	0.01095	0.13456
53	H	0.2286	0.24055	0.21773	0.01195	0.01087	0.01141
54	H	0.22707	0.23238	0.22049	0.00531	0.00658	0.005945
55	H	0.22829	0.23591	0.21989	0.00762	0.0084	0.00801
56	H	0.25435	0.26682	0.25108	0.01247	0.00327	0.00787
57	H	0.26001	0.25852	0.2595	-0.00149	0.00051	-0.00049
58	H	0.25148	0.26344	0.24317	0.01196	0.00831	0.010135
59	H	0.24747	0.26477	0.23827	0.0173	0.0092	0.01325
60	H	0.21894	0.22543	0.21778	0.00649	0.00116	0.003825

61	H	0.25323	0.25023	0.25054	-0.003	0.00269	-0.000155
62	H	0.51987	0.52424	0.51875	0.00437	0.00112	0.002745
63	H	0.24487	0.25089	0.22964	0.00602	0.01523	0.010625
64	H	0.50463	0.51079	0.45143	0.00616	0.0532	0.02968
65	H	0.22247	0.23198	0.20436	0.00951	0.01811	0.01381
66	H	0.50581	0.50961	0.49573	0.0038	0.01008	0.00694
67	H	0.25546	0.26224	0.24246	0.00678	0.013	0.00989
68	H	0.22574	0.22332	0.2238	-0.00242	0.00194	-0.00024
69	H	0.20599	0.21354	0.19705	0.00755	0.00894	0.008245
70	H	0.50041	0.50375	0.49164	0.00334	0.00877	0.006055