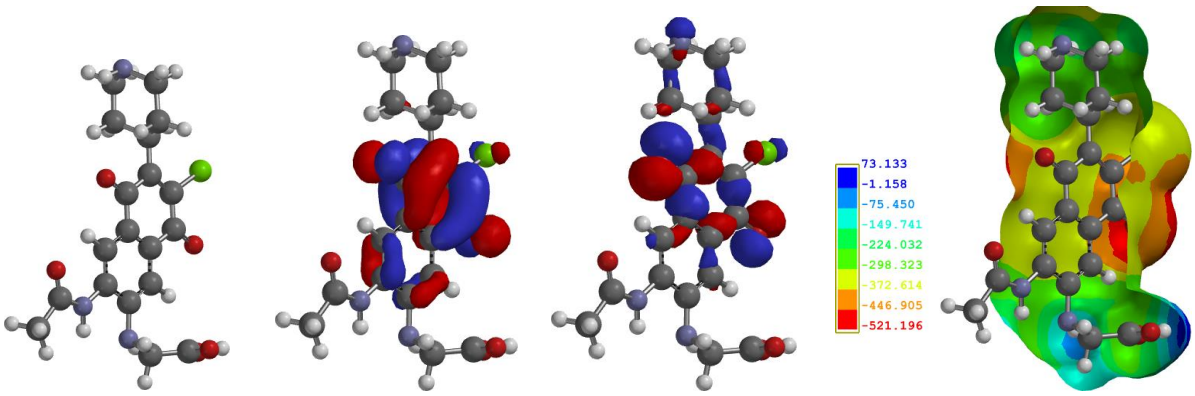
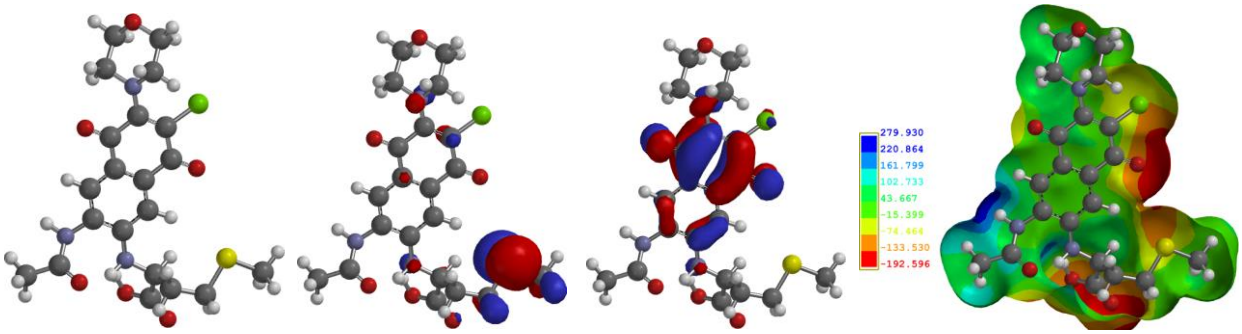
Supplementary File

Supporting Information: 'Corrosion Inhibitive Potentials of Some Amino Acid Derivatives of 1,4-Naphthoquinone–DFT Calculations'



(a) **(b)** **(c)** **(d)**

Figure S1. (a) The structure Optimized (b) Highest Occupied Molecular Orbital map and (c) Lowest Unoccupied Molecular Orbital map of B.



(a) (b) (c) (d)

Figure S2. (a) The structure Optimized (b) Highest Occupied Molecular Orbital map and (c) Lowest Unoccupied Molecular Orbital map of C.

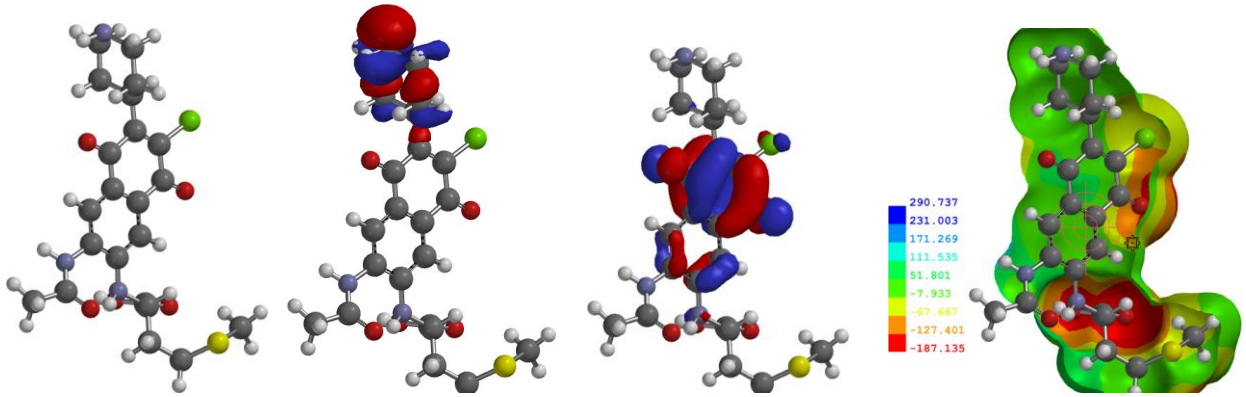


Figure S3. (a) The structure Optimized (b) Highest Occupied Molecular Orbital map and (c) Lowest Unoccupied Molecular Orbital map of D.

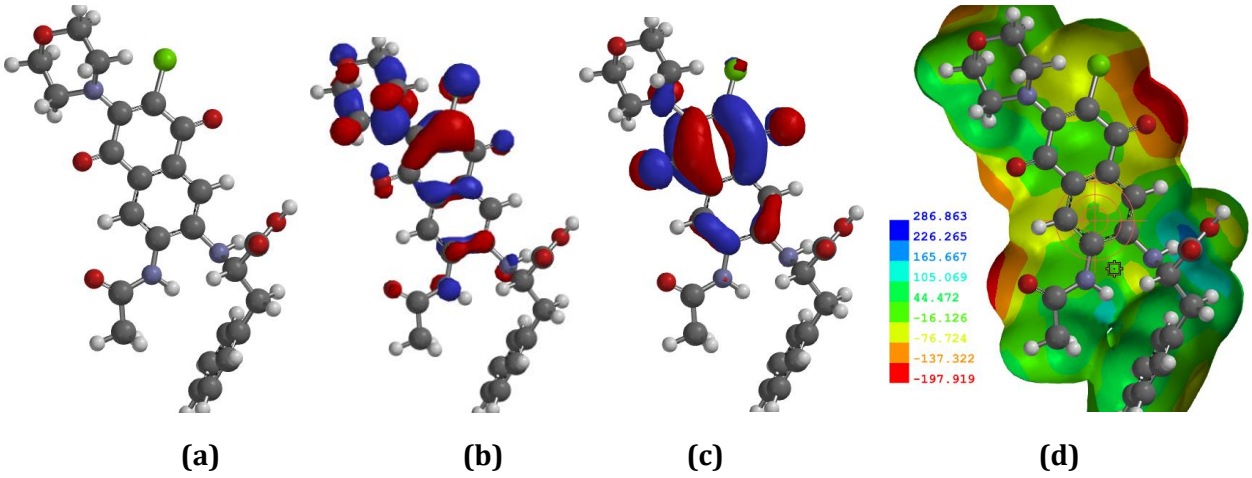


Figure S4. (a) The structure Optimized (b) Highest Occupied Molecular Orbital map and (c) Lowest Unoccupied Molecular Orbital map of E.

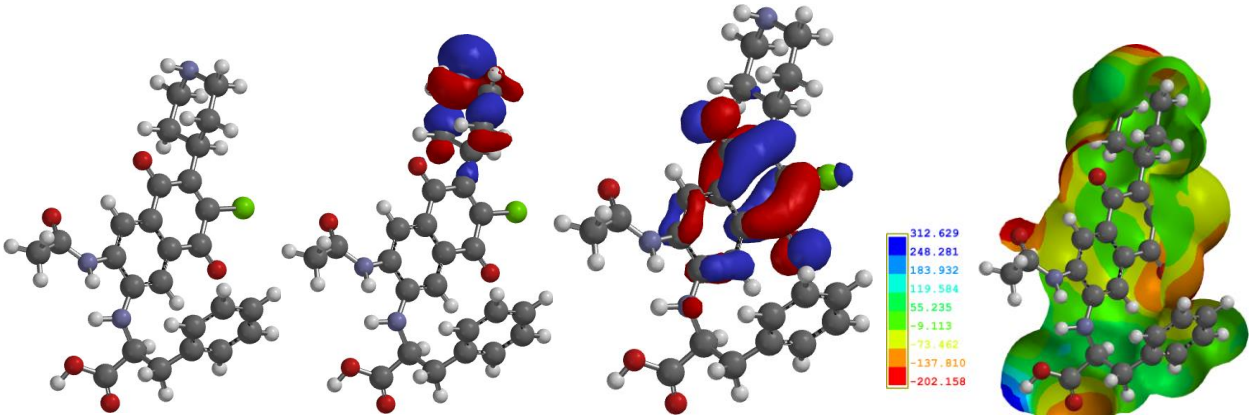


Figure S5. (a) The structure Optimized (b) Highest Occupied Molecular Orbital map and (c) Lowest Unoccupied Molecular Orbital map of F.

Table S1. The selected Calculated Mulliken atomic charges and Fukui functions of compound B.

S/N	Atom	qK(N+1)	Qk	qk(N-1)	f_k^+	f_k^-	Δfk
1	C0	0.579	0.577	0.587	0.002	-0.01	0.012
2	N1	-0.652	-0.652	-0.633	0	-0.019	0.019
3	C2	-0.224	-0.242	-0.27	0.018	0.028	-0.01
4	O3	-0.461	-0.44	-0.411	-0.021	-0.029	0.008
5	O4	-0.583	-0.567	-0.568	-0.016	0.001	-0.017
6	C5	-0.268	-0.246	-0.238	-0.022	-0.008	-0.014
7	C6	0.201	0.229	-0.293	-0.028	**0.522**	**-0.55**
8	C7	0.331	0.356	0.368	-0.025	-0.012	-0.013
9	C8	-0.255	-0.237	-0.224	-0.018	-0.013	-0.005
10	C9	0.059	0.063	0.68	-0.004	-0.005	0.001
11	C10	0.3	0.36	0.371	-0.06	-0.011	-0.049
12	C11	0.104	0.137	0.124	-0.033	0.013	-0.046
13	C12	-0.262	-0.249	-0.241	-0.013	-0.008	-0.005
14	C13	0.375	0.42	0.427	-0.045	-0.007	-0.038
15	C14	0.046	0.053	0.063	-0.007	-0.01	0.003
16	O15	-0.582	-0.458	-0.424	-0.124	-0.034	-0.09
17	O16	-0.594	-0.467	-0.468	-0.127	0.001	-0.128
18	N17	-0.537	-0.523	-0.417	-0.014	-0.106	0.092
10	C18	-0.147	-0.152	-0.176	0.005	0.024	-0.019
20	C19	-0.27	-0.28	-0.29	0.01	0.01	0
21	C20	-0.149	-0.171	-0.185	**0.022**	0.014	**0.008**
22	C21	-0.27	-0.28	-0.29	0.01	0.01	0
23	C22	-0.148	-0.153	-0.177	0.005	0.024	-0.019
24	Cl23	-0.094	0.034	0.092	-0.128	-0.058	-0.07
25	N24	-0.723	-0.731	-0.722	0.008	-0.009	0.017
26	C25	0.596	0.601	0.603	-0.005	-0.002	-0.003
27	C26	-0.502	-0.472	-0.436	-0.03	-0.036	0.006
28	C27	-0.537	-0.546	-0.558	0.009	0.012	-0.003

Table S2. The selected Calculated Mulliken atomic charges and Fukui functions of compound C.

Atom	qK(N+1)	Qk	qk(N-1)	f_k^+	f_k^-	Δfk
C0	0.605	0.607	0.62	-0.002	-0.013	0.011
N1	-0.781	-0.784	-0.747	0.003	-0.037	0.04
C2	-0.054	-0.247	-0.087	**0.193**	-0.16	**0.353**
C3	-0.266	-0.283	-0.283	0.017	0	0.017
C4	-0.427	0.417	-0.443	-0.844	**0.86**	**-1.704**
S5	0.053	0.082	0.181	-0.029	-0.099	0.07
C6	-0.594	-0.587	-0.604	-0.007	0.017	-0.024
O7	-0.497	-0.457	-0.426	-0.04	-0.031	-0.009
O8	-0.58	-0.573	-0.549	-0.007	-0.024	0.017
C9	-0.26	-0.269	-0.26	0.009	-0.009	0.018
C10	0.299	0.351	0.381	-0.052	-0.03	-0.022
C11	0.306	0.317	0.363	-0.011	-0.046	0.035
C12	-0.286	-0.26	-0.266	-0.026	0.006	-0.032
C13	0.06	0.054	0.063	0.006	-0.009	0.015
C14	0.334	0.363	0.378	-0.029	-0.015	-0.014
C15	0.174	0.307	0.318	-0.133	-0.011	-0.122
C16	-0.217	-0.255	-0.235	0.038	-0.02	0.058
C17	0.36	0.413	0.424	-0.053	-0.011	-0.042
C18	0.052	0.05	0.067	0.002	-0.017	0.019
O19	-0.56	-0.461	-0.434	-0.099	-0.027	-0.072
O20	-0.602	-0.481	-0.463	-0.121	-0.018	-0.103
N21	-0.473	-0.471	-0.438	-0.002	-0.033	0.031
C22	-0.12	-0.161	-0.188	0.041	0.027	0.014
C23	-0.031	-0.035	-0.046	0.004	0.011	-0.007
O24	-0.484	-0.466	-0.434	-0.018	-0.032	0.014
C25	-0.031	-0.118	-0.049	0.087	-0.069	0.156
C26	-0.119	-0.134	-0.167	0.015	0.033	-0.018
CI27	-0.065	0.02	0.116	-0.085	-0.096	0.011
N28	-0.695	-0.69	-0.707	-0.005	0.017	-0.022
C29	0.587	0.588	0.594	-0.001	-0.006	0.005
O30	-0.527	-0.511	-0.489	-0.016	-0.022	0.006
C31	-0.533	-0.531	-0.549	-0.002	0.018	-0.02

Table S3. The selected Calculated Mulliken atomic charges and Fukui functions of compound D.

S/N	Atom	qk(N+1)	qk(N)	qk(N-1)	f_k^+	f_k^-	Δfk
1	C0	0.605	0.613	0.62	-0.008	-0.007	-0.001
2	N1	-0.78	-0.786	-0.754	0.006	-0.032	0.038
3	C2	-0.051	-0.046	-0.082	-0.005	0.036	-0.041
4	C3	-0.271	-0.301	-0.286	0.03	-0.015	0.045
5	C4	-0.426	-0.431	-0.449	0.005	0.018	-0.013
6	S5	0.049	0.069	0.215	-0.02	-0.146	0.126
7	C6	-0.594	-0.603	-0.609	0.009	0.006	0.003
8	O7	-0.497	-0.461	-0.432	-0.036	-0.029	-0.007
9	O8	-0.581	-0.57	-0.55	-0.011	-0.02	0.009
10	C9	-0.258	-0.256	-0.254	-0.002	-0.002	0
11	C10	0.291	0.346	0.368	-0.055	-0.022	-0.033
12	C11	0.307	0.325	0.349	-0.018	-0.024	0.006
13	C12	-0.283	-0.265	-0.264	-0.018	-0.001	-0.017
14	C13	0.073	0.07	0.076	0.003	-0.006	0.009
15	C14	0.301	0.357	0.364	-0.056	-0.007	-0.049
16	C15	0.106	0.138	0.128	-0.032	0.01	-0.042
17	C16	-0.261	0.357	-0.243	-0.618	0.6	-1.218
18	C17	0.375	0.138	0.426	0.237	-0.288	0.525
19	C18	0.046	-0.249	0.051	0.295	-0.3	0.595
20	O19	-0.562	0.424	-0.427	-0.986	0.851	-1.837
21	O20	-0.607	0.049	-0.482	-0.656	0.531	-1.187
22	N21	-0.536	-0.441	-0.439	-0.095	-0.002	-0.093
23	C22	-0.148	-0.486	-0.17	0.338	-0.316	0.654
24	C23	-0.271	-0.523	-0.286	0.252	-0.237	0.489
25	C24	-0.149	-0.153	-0.184	0.004	0.031	-0.027
26	C25	-0.27	-0.278	-0.286	0.008	0.008	0
27	C26	-0.148	-0.172	-0.171	0.024	-0.001	0.025
28	Cl27	-0.079	-0.279	0.083	0.2	-0.362	0.562
29	N28	-0.694	-0.153	-0.703	-0.541	0.55	-1.091
30	C29	0.589	0.042	0.591	**0.547**	-0.549	**1.096**
31	O30	-0.527	-0.701	-0.497	0.174	-0.204	0.378
32	C31	-0.534	0.59	-0.547	-1.124	**1.137**	**-1.714**

Table S4. The selected Calculated Mulliken atomic charges and Fukui functions of compound E.

S/N	Atom	qk(N+1)	qk(N)	qk(N-1)	f_k^+	f_k^-	Δfk
1	C0	0.893	0.581	0.594	0.312	-0.013	0.325
2	N1	-0.799	-0.664	-0.639	-0.135	-0.025	-0.11
3	C2	-0.134	-0.053	-0.093	-0.081	**0.04**	**-0.121**
4	C3	-0.422	-0.38	-0.375	-0.042	-0.005	-0.037
5	C4	-0.049	0.169	0.151	-0.218	0.018	-0.236
6	C5	-0.231	-0.186	-0.151	-0.045	-0.035	-0.01
7	C6	-0.236	-0.131	-0.13	-0.105	-0.001	-0.104
8	C7	-0.245	-0.129	-0.129	-0.116	0	-0.116
9	C8	-0.239	-0.137	-0.133	-0.102	-0.004	-0.098
10	C9	-0.222	-0.177	-0.195	-0.045	0.018	-0.063
11	O10	-0.603	-0.484	-0.421	-0.119	-0.063	-0.056
12	O11	-0.726	-0.575	-0.577	-0.151	0.002	-0.153
13	C12	-0.188	-0.257	-0.252	0.069	-0.005	0.074
14	C13	0.162	0.244	0.321	-0.082	-0.077	-0.005
15	C14	0.395	0.356	0.373	0.039	-0.017	0.056
16	C15	-0.201	-0.239	-0.226	0.038	-0.013	0.051
17	C16	-0.123	0.05	0.058	-0.173	-0.008	-0.165
18	C17	0.441	0.364	0.381	0.077	-0.017	0.094
19	C18	0.235	0.302	0.319	-0.067	-0.017	-0.05
20	C19	-0.254	-0.251	-0.229	-0.003	-0.022	0.019
21	C20	0.486	0.416	0.443	0.07	-0.027	0.097
22	C21	-0.161	0.061	0.077	-0.222	-0.016	-0.206
23	O22	-0.647	-0.479	-0.44	-0.168	-0.039	-0.129
24	O23	-0.645	-0.466	-0.443	-0.179	-0.023	-0.156
25	N24	-0.759	-0.481	-0.429	-0.278	-0.052	-0.226
26	C25	-0.199	-0.158	-0.192	-0.041	0.034	-0.075
27	C26	-0.199	-0.034	-0.047	-0.165	0.013	-0.178
28	O27	-0.65	-0.467	-0.431	-0.183	-0.036	-0.147
29	C28	-0.08	-0.038	-0.051	-0.042	0.013	-0.055
30	C29	-0.198	-0.131	-0.172	-0.067	0.041	-0.108
31	Cl30	-0.083	0.015	0.13	-0.098	-0.115	0.017
32	N31	-1.083	-0.74	-0.736	-0.343	-0.004	-0.339
33	C32	0.847	0.593	0.6	0.254	-0.007	0.261
34	O33	-0.627	-0.475	-0.435	-0.152	-0.04	-0.112
35	C34	-0.053	-0.551	-0.559	**0.498**	0.008	**0.49**

Table S5. The selected Calculated Mulliken atomic charges and Fukui functions of compound F.

S/N	Atom	qK(N+1)	Qk	qk(N-1)	f_k^+	f_k^-	Δfk
1	C0	0.576	0.588	0.602	1.164	-0.014	1.178
2	N1	-0.698	-0.722	-0.686	-1.42	-0.036	-1.384
3	C2	-0.007	-0.041	-0.057	-0.048	0.016	-0.064
4	C3	-0.356	-0.35	-0.365	-0.706	0.015	-0.721
5	C4	0.144	0.165	0.166	0.309	-0.001	0.31
6	C5	-0.178	-0.188	-0.192	-0.366	0.004	-0.37
7	C6	-0.132	-0.117	-0.117	-0.249	0	-0.249
8	C7	-0.131	-0.129	-0.128	-0.26	-0.001	-0.259
9	C8	-0.185	-0.128	-0.127	-0.313	-0.001	-0.312
10	C9	-0.468	-0.168	-0.183	-0.636	0.015	-0.651
11	O10	-0.574	-0.449	-0.419	-1.023	-0.03	-0.993
12	O11	-0.574	-0.582	-0.587	-1.156	0.005	-1.161
13	C12	-0.256	-0.243	-0.22	-0.499	-0.023	-0.476
14	C13	0.192	0.341	0.381	0.533	-0.04	0.573
15	C14	0.336	0.312	0.35	0.648	-0.038	0.686
16	C15	-0.263	-0.217	-0.206	-0.48	-0.011	-0.469
17	C16	0.061	0.051	0.063	0.112	-0.012	0.124
18	C17	0.299	0.355	0.368	0.654	-0.013	0.667
19	C18	0.105	0.138	0.131	0.243	0.007	0.236
20	C19	-0.263	-0.25	-0.244	-0.513	-0.006	-0.507
21	C20	0.376	0.42	0.431	0.796	-0.011	0.807
22	C21	0.04	0.049	0.056	0.089	-0.007	0.096
23	O22	-0.578	-0.457	-0.429	-1.035	-0.028	-1.007
24	O23	-0.592	-0.48	-0.467	-1.072	-0.013	-1.059
25	N24	-0.537	-0.524	-0.446	-1.061	-0.078	-0.983
26	C25	-0.147	-0.152	-0.17	-0.299	0.018	-0.317
27	C26	-0.271	-0.28	-0.288	-0.551	0.008	-0.559
28	C27	-0.149	-0.169	-0.169	-0.318	0	-0.318
29	C28	-0.27	-0.28	0.086	-0.55	-0.366	-0.184
30	C29	-0.148	-0.153	-0.742	-0.301	**0.589**	**-0.89**
31	Cl30	-0.09	0.027	0.602	-0.063	-0.575	0.512
32	N31	-0.724	-0.739	-0.439	-1.463	-0.3	-1.163
33	C32	0.596	0.597	0.602	**1.193**	-0.005	**1.198**