

Supporting Information (SI)

Green inhibitor of Carbon steel corrosion in 1 M hydrochloric acid: *Eruca sativa* seeds extract (Experimental and Theoretical studies)

Weight loss results:

Table S1

Weight loss measurements of carbon steel in 1M HCl solution containing various concentrations of *eruca sativa* seeds extract after immersion time for 90min at 25, 35 °C,

Conc. , g/L	25 °C				35 °C			
	Δm mgcm ⁻²	θ	%I E	C.R. mg cm ⁻² min ⁻¹	Δw mgcm ⁻²	θ	%I E	C.R. mg cm ⁻² min ⁻¹
Blank	22.81±0.00 4			0.3802	25.30±0.00 3			0.4209
0.05	3.43±0.002	0.85 0	85.0	0.0571	7.83±0.001	0.69 0	69.0	0.1305 2
0.10	2.98±0.001	0.87 0	87.0	0.0496	7.66±0.002	0.69 7	69.7	0.1276 0
0.15	2.28±0.003	0.90 0	90.0	0.0378 8	6.74±0.001	0.73 3	73.3	0.1122 7
0.20	1.84±0.001	0.91 9	91.9	0.0306 1	5.05±0.003	0.80 0	80.0	0.0842 1
0.25	1.39±0.001	0.93 9	93.9	0.0232 1	4.61±0.001	0.81 7	81.7	0.0768 4
0.30	1.184±0.00 2	0.94 8	94.8	0.0197 3	3.34±0.002	0.86 8	86.8	0.0557 0

Table S2

Conc., Ppm	45 °C				55 °C			
	Δw mgcm^{-2}	θ	%IE	C.R. $\text{mg cm}^{-2}\text{min}^{-1}$	Δw mgcm^{-2}	θ	%IE	C.R. $\text{mg cm}^{-2}\text{min}^{-1}$
Blank	26.39±0.002			0.4365	27.43±0.005			0.4630
0.05	13.49±0.001	0.447	44.7	0.2248	17.13±0.003	0.383	38.3	0.2856
0.10	13.34±0.003	0.453	45.3	0.2223	16.26±0.002	0.415	41.5	0.2710
0.15	12.27±0.002	0.497	49.7	0.2045	15.20±0.002	0.453	45.3	0.2533
0.20	10.76±0.004	0.559	55.9	0.1794	12.46±0.001	0.552	55.2	0.2076
0.25	9.45±0.002	0.613	61.3	0.1575	10.97±0.001	0.605	60.5	0.1828
0.30	8.48±0.003	0.652	65.2	0.1413	10.11±0.002	0.636	63.6	0.1690

Weight loss measurements of carbon steel in 1M HCl solution containing various concentrations of eruca sativa seeds extract after immersion time for 90min at 45, 55 °C,

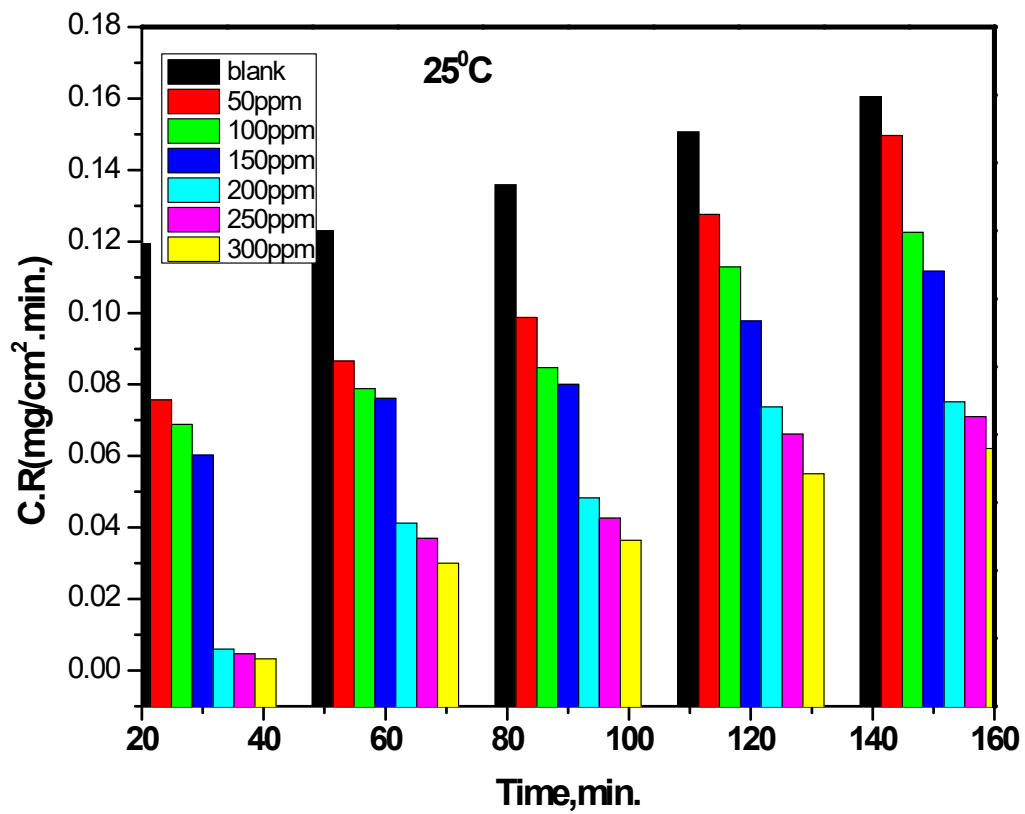


Figure S1 depicts the corrosion rate of a carbon steel electrode dipped in a 1 M HCl solution containing various concentrations of eruca sativa seeds extract at 25°C as a function of time.

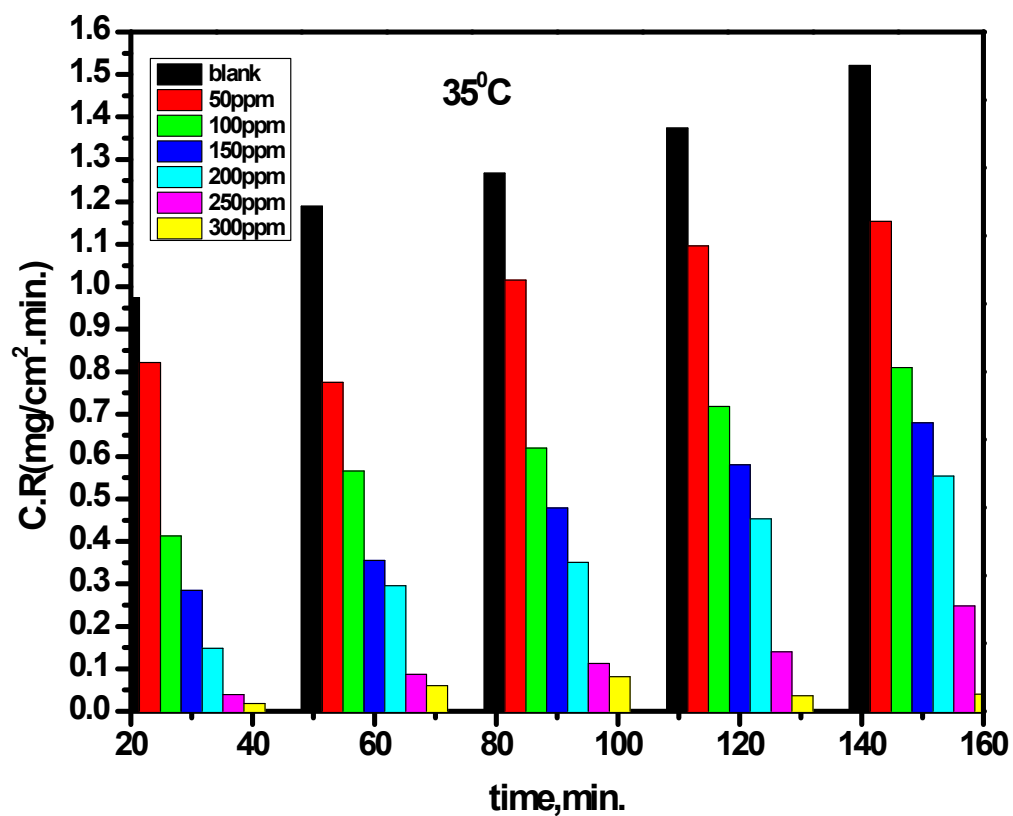


Figure S2 depicts the corrosion rate of a carbon steel electrode dipped in a 1 M HCl solution containing various concentrations of eruca sativa seeds extract at 35°C as a function of time.

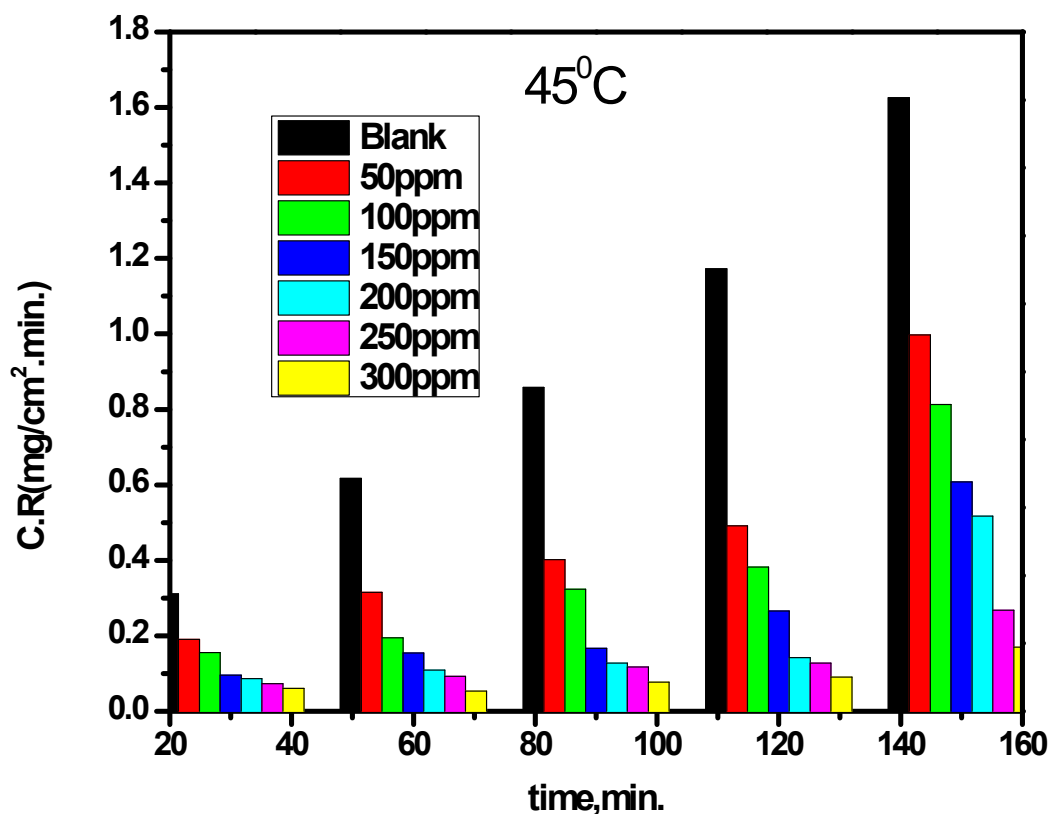


Figure S3 depicts the corrosion rate of a carbon steel electrode dipped in a 1 M HCl solution containing various concentrations of eruca sativa seeds extract at 45°C as a function of time.

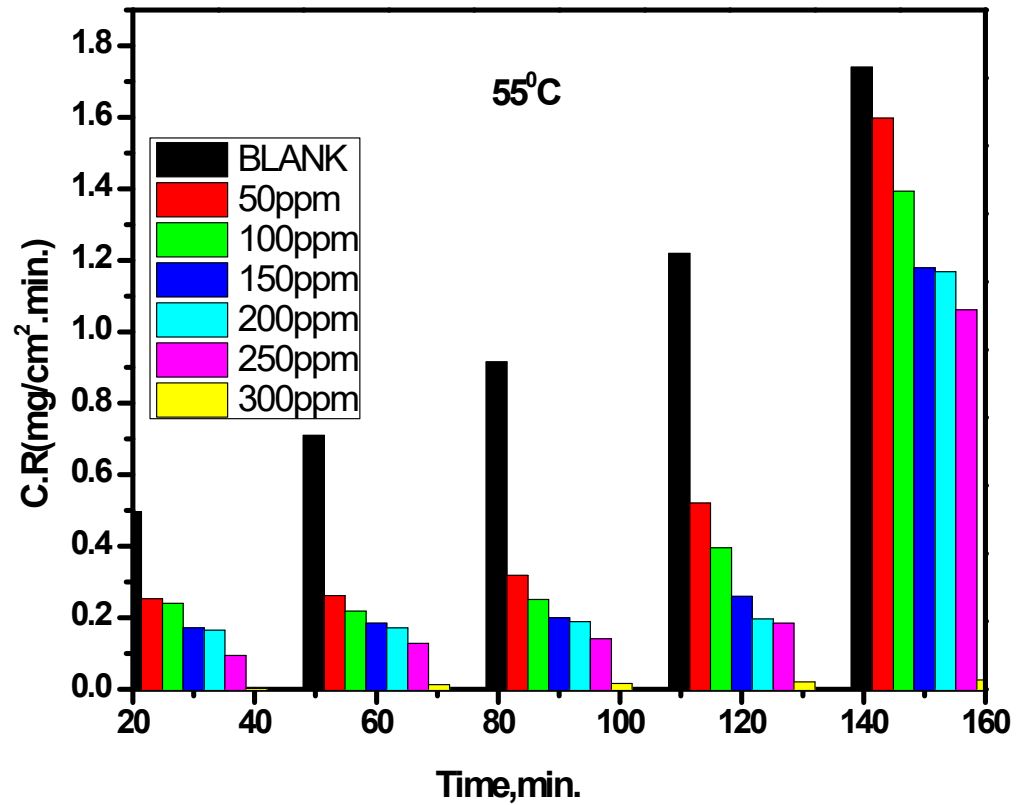


Figure S4 depicts the corrosion rate of a carbon steel electrode dipped in a 1 M HCl solution containing various concentrations of eruca sativa seeds extract at 55°C as a function of time

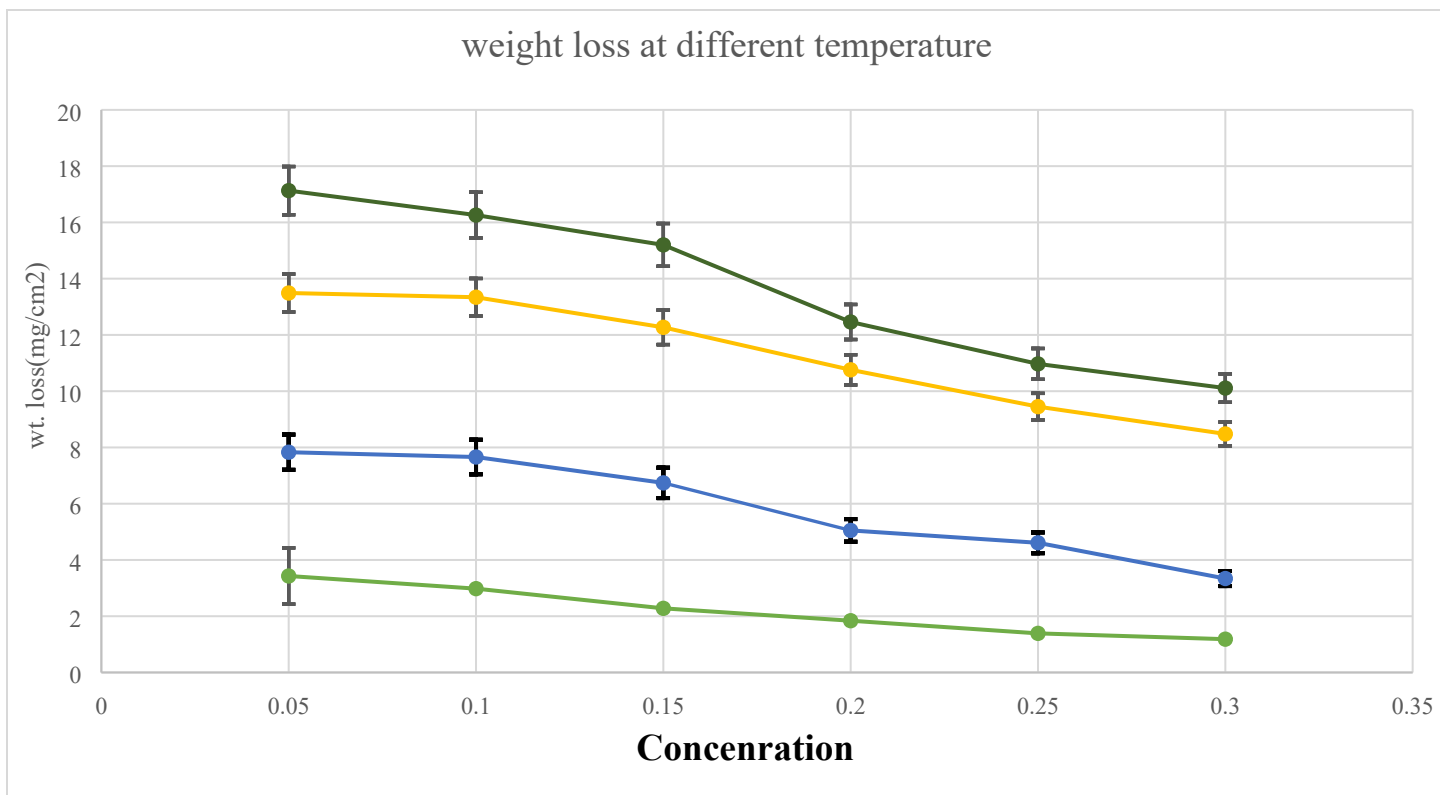


Fig. S5. Standard deviation of weight loss results of carbon steel electrode dipped in 1 M HCl solution with different concentrations (0.05-0.30g/L) of eruca sativa seeds, after a 90-minute immersion time at various temperatures (25-55°C)..

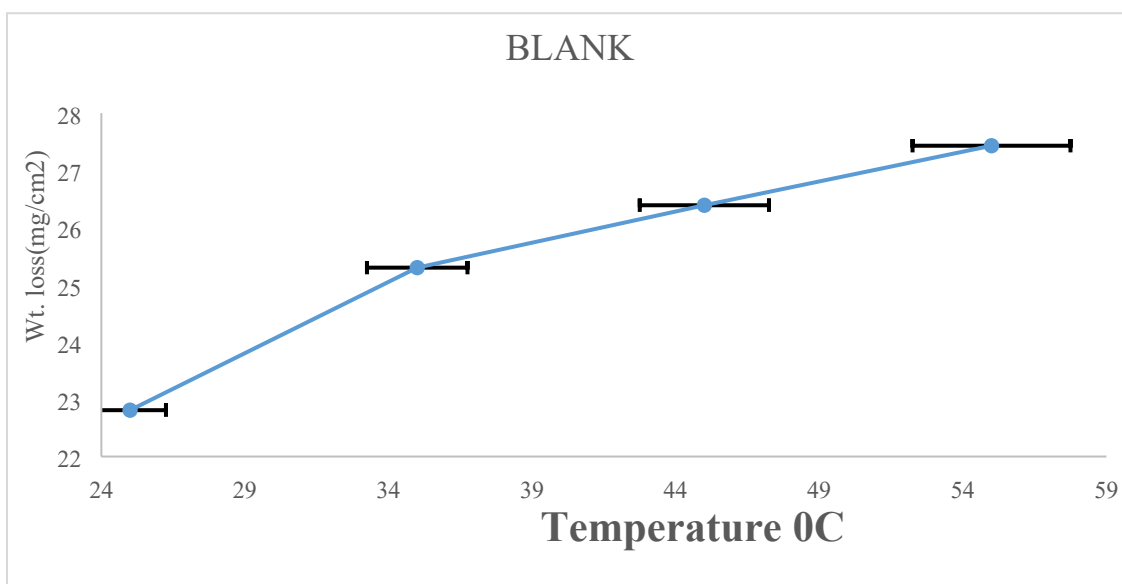


Fig. S6. Standard deviation of weight loss results of carbon steel electrode dipped in 1 M HCl solution without different concentrations of eruca sativa seeds, after a 90-minute immersion time at various temperatures (25-55°C).

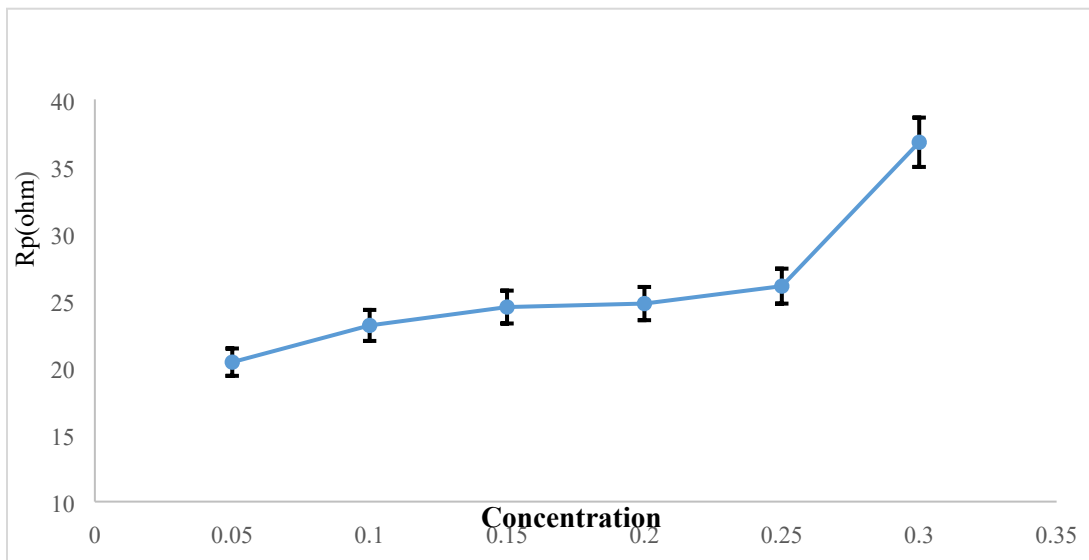


Fig. S7. Standard deviation of resistance polarization results of carbon steel electrode dipped in 1 M HCl solution with different concentrations (0.05-0.30g/L) of eruca sativa seeds, at (25°C)..

Adsorption isotherms

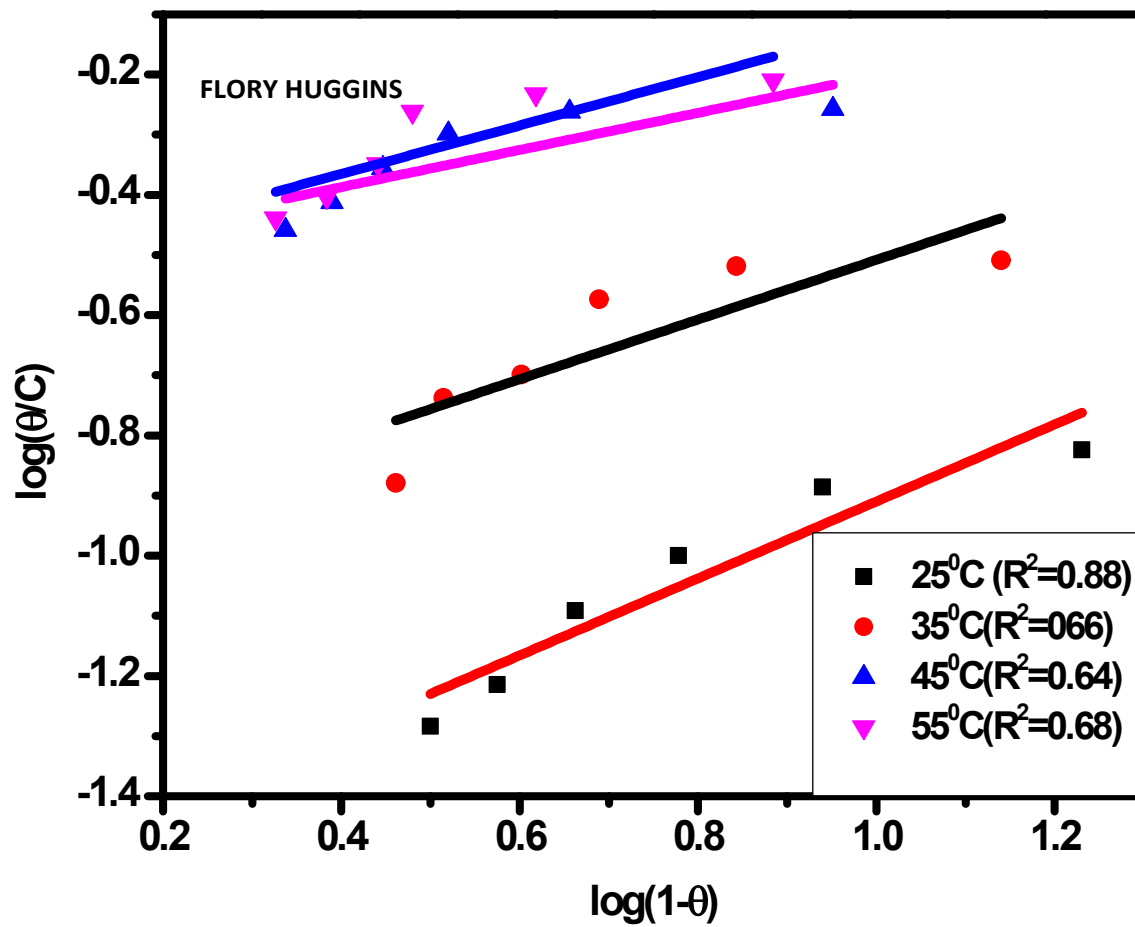


Fig. S8. Flory- Huggins adsorption isotherm plotted as $\log\theta/C$ vs. $\log(1-\theta)$ of eruca sativa seeds extract for corrosion of carbon steel in 1 M HCl solution at 25 °C.

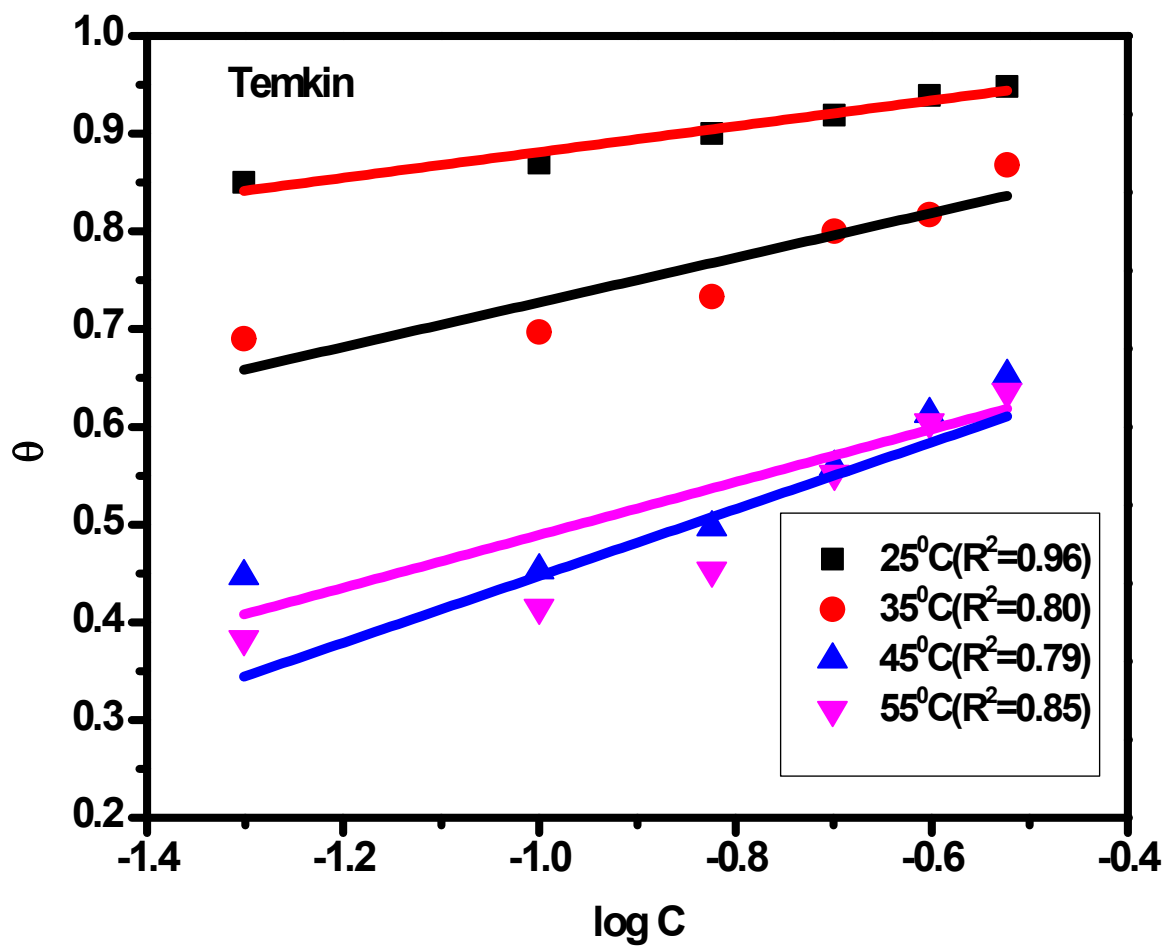


Fig. S9. Temkin adsorption isotherm plotted as θ vs. $\log C$ of eruca sativa seeds extract for corrosion of carbon steel in 1 M HCl solution at 25 °C.

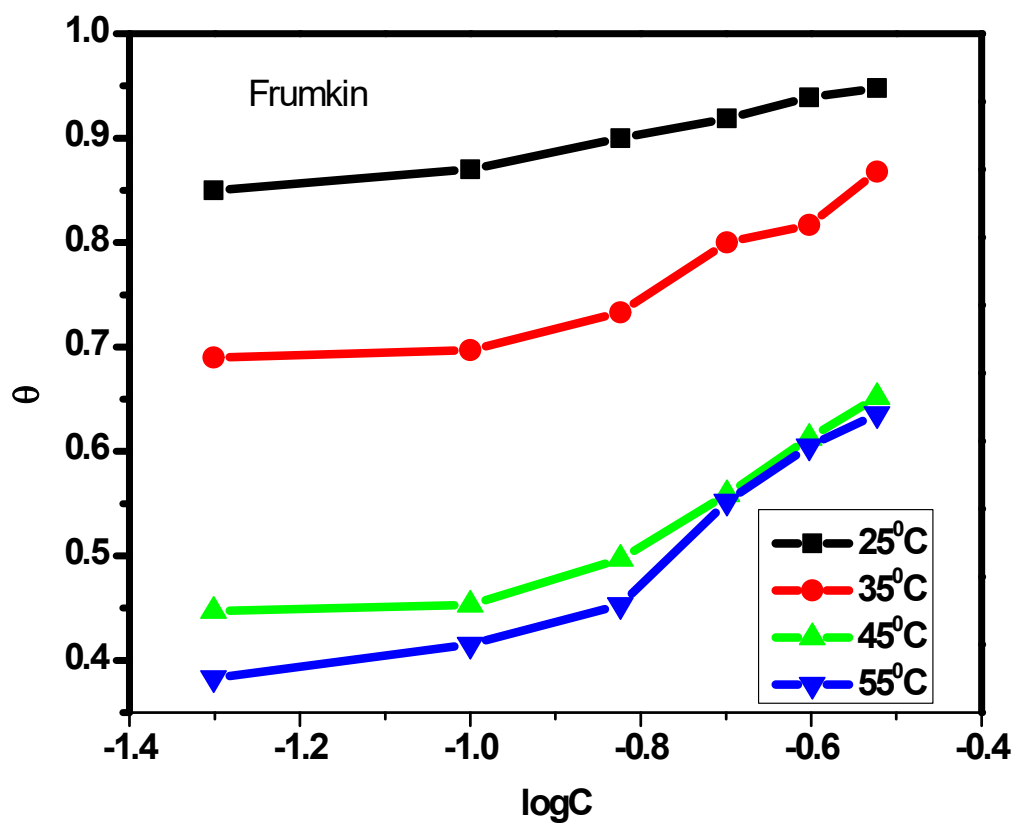


Fig. S10. Frumkin adsorption isotherm plotted as θ vs. $\log C$ of eruca sativa seeds extract for corrosion of carbon steel in 1 M HCl solution at 25 °C.

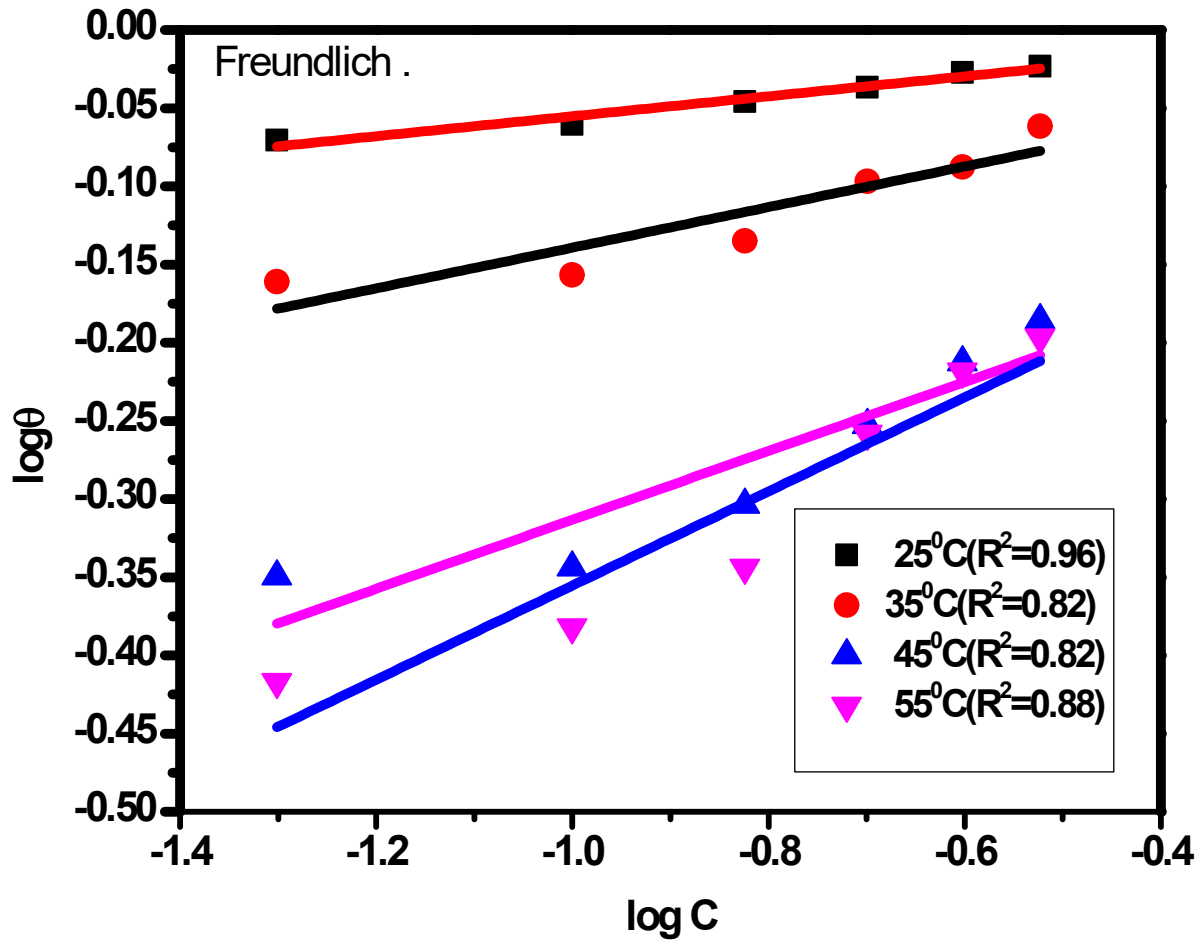


Fig. S11. Freundlich adsorption isotherm plotted as log θ vs. log C of eruca sativa seeds extract for corrosion of carbon steel in 1 M HCl solution at 25 °C.

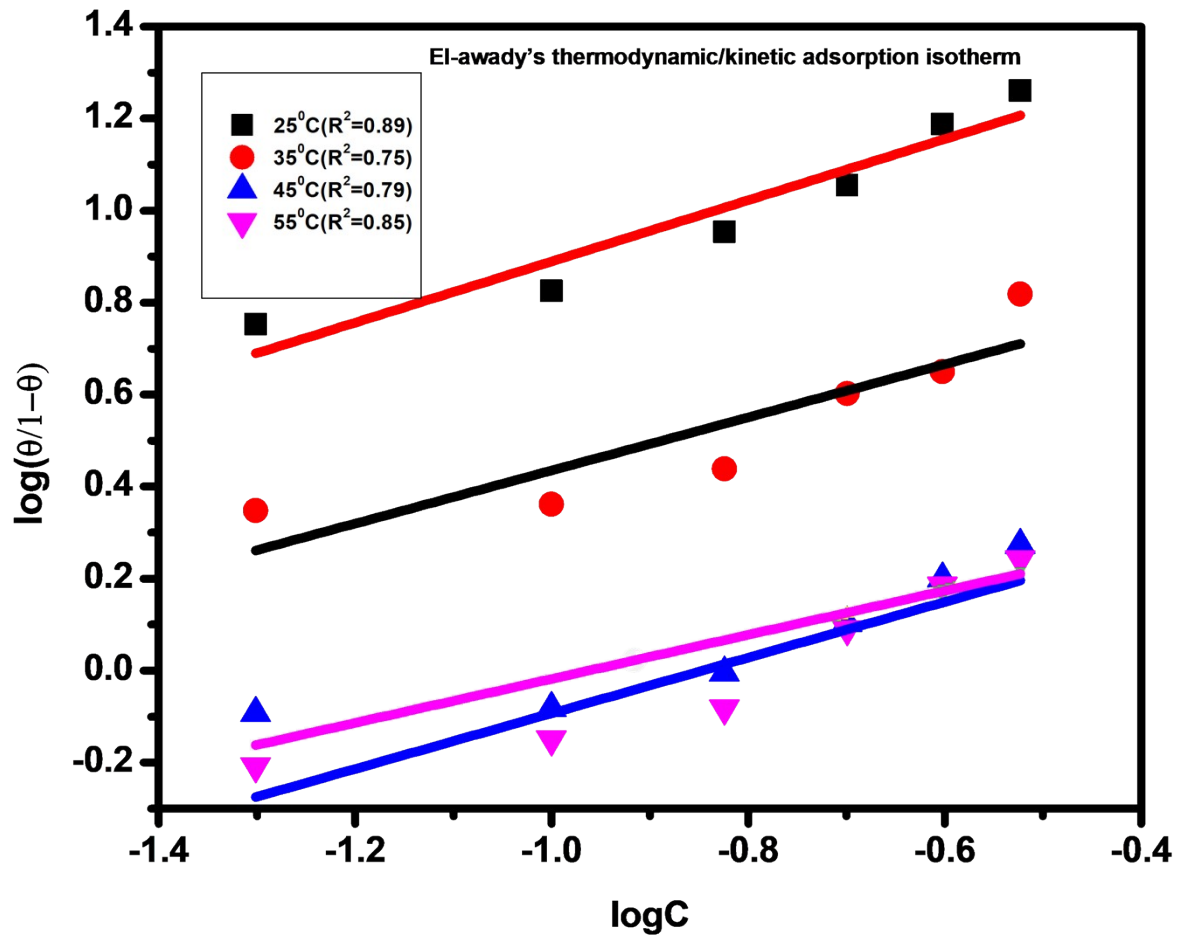


Fig. S12. Elawady s adsorption isotherm plotted as $\log(\theta/1-\theta)$ vs. $\log C$ of eruca sativa seeds extract for corrosion of carbon steel in 1 M HCl solution at 25 °C.

TableS3

Quercetin(neutral)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.104	0.078
C (2)	0.026	0.046
O (3)	0.029	0.032
C (4)	0.112	0.096
O (5)	0.120	0.121
C (6)	0.005	0.024
C (7)	0.050	0.040
O (8)	0.027	0.031
C (9)	0.028	0.032
C (10)	0.031	0.038
O (11)	0.028	0.030
C (12)	0.034	0.032
C (13)	0.021	0.026
O (14)	0.039	0.049
C (15)	0.007	0.020
C (16)	0.028	0.027
C (17)	0.014	0.017
O (18)	0.022	0.010
C (19)	0.024	0.031
O (20)	0.026	0.030
C (21)	0.018	0.022
C (22)	0.016	0.028
H (23)	0.020	0.015
H (24)	0.014	0.014
H (25)	0.028	0.017
H (26)	0.011	0.012
H (27)	0.029	0.019
H (28)	0.027	0.013
H (29)	0.003	0.003
H (30)	0.007	0.019
H (31)	0.021	0.013
H (32)	0.030	0.017

Mulliken atomic charges:

	charge	spin
C (1)	0.264	0.000
C (2)	0.223	0.000
O (3)	-0.503	0.000
C (4)	0.316	0.000
O (5)	-0.578	0.000
C (6)	-0.058	0.000
C (7)	0.318	0.000
O (8)	-0.468	0.000
C (9)	-0.171	0.000
C (10)	0.354	0.000
O (11)	-0.478	0.000
C (12)	-0.177	0.000
C (13)	0.330	0.000
O (14)	-0.494	0.000
C (15)	0.014	0.000

C (16)	-0.085	0.000
C (17)	0.283	0.000
O (18)	-0.545	0.000
C (19)	0.308	0.000
O (20)	-0.484	0.000
C (21)	-0.084	0.000
C (22)	-0.080	0.000
H (23)	0.272	0.000
H (24)	0.285	0.000
H (25)	0.062	0.000
H (26)	0.291	0.000
H (27)	0.052	0.000
H (28)	0.049	0.000
H (29)	0.303	0.000
H (30)	0.286	0.000
H (31)	0.050	0.000
H (32)	0.049	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.053	0.063
C (2)	0.087	0.081
O (3)	0.102	0.096
C (4)	0.026	0.030
O (5)	0.065	0.061
C (6)	0.020	0.020
C (7)	0.032	0.033
O (8)	0.035	0.037
C (9)	0.034	0.033
C (10)	0.019	0.030
O (11)	0.028	0.029
C (12)	0.058	0.058
C (13)	0.014	0.019
O (14)	0.046	0.046
C (15)	0.002	0.023
C (16)	0.033	0.028
C (17)	0.018	0.023
O (18)	0.001	0.016
C (19)	0.041	0.035
O (20)	0.037	0.033
C (21)	0.019	0.026
C (22)	0.028	0.025
H (23)	0.025	0.030
H (24)	0.015	0.016
H (25)	0.026	0.017
H (26)	0.011	0.012
H (27)	0.036	0.023
H (28)	0.023	0.017
H (29)	0.012	0.012
H (30)	0.013	0.002
H (31)	0.023	0.015
H (32)	0.020	0.012

Quercetin(protonated)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.096	0.075
C (2)	0.037	0.050
O (3)	0.036	0.036
C (4)	0.128	0.114
O (5)	0.140	0.140
C (6)	0.001	0.026
C (7)	0.048	0.038
O (8)	0.028	0.032
C (9)	0.024	0.029
C (10)	0.040	0.046
O (11)	0.036	0.038
C (12)	0.030	0.031

C (13)	0.043	0.034
O (14)	0.013	0.026
C (15)	-0.009	0.011
C (16)	0.021	0.021
C (17)	0.014	0.015
O (18)	0.017	0.012
C (19)	0.020	0.023
O (20)	0.019	0.020
C (21)	0.014	0.018
C (22)	0.018	0.021
H (23)	0.017	0.016
H (24)	0.015	0.015
H (25)	0.027	0.017
H (26)	0.013	0.014
H (27)	0.028	0.018
H (28)	0.019	0.018
H (29)	0.021	0.012
H (30)	0.004	0.005
H (31)	0.003	0.008
H (32)	0.017	0.011
H (33)	0.022	0.012

Mulliken atomic charges:

	charge	spin
C (1)	0.250	0.000
C (2)	0.276	0.000
O (3)	-0.464	0.000
C (4)	0.338	0.000
O (5)	-0.498	0.000
C (6)	-0.032	0.000
C (7)	0.337	0.000
O (8)	-0.444	0.000
C (9)	-0.146	0.000
C (10)	0.365	0.000
O (11)	-0.450	0.000
C (12)	-0.152	0.000
C (13)	0.351	0.000
O (14)	-0.429	0.000
C (15)	-0.014	0.000
C (16)	-0.077	0.000
C (17)	0.295	0.000
O (18)	-0.523	0.000
C (19)	0.314	0.000
O (20)	-0.469	0.000
C (21)	-0.070	0.000
C (22)	-0.055	0.000
H (23)	0.286	0.000
H (24)	0.297	0.000
H (25)	0.081	0.000
H (26)	0.301	0.000
H (27)	0.092	0.000
H (28)	0.367	0.000
H (29)	0.064	0.000
H (30)	0.302	0.000
H (31)	0.292	0.000
H (32)	0.060	0.000
H (33)	0.057	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.044	0.038
C (2)	0.050	0.051
O (3)	0.064	0.062
C (4)	0.015	0.016
O (5)	0.036	0.035
C (6)	0.015	0.016
C (7)	0.014	0.015
O (8)	0.017	0.018
C (9)	0.014	0.012

C (10)	0.010	0.015
O (11)	0.018	0.018
C (12)	0.024	0.024
C (13)	0.006	0.009
O (14)	0.000	0.013
C (15)	0.040	0.061
C (16)	0.040	0.037
C (17)	0.051	0.056
O (18)	0.041	0.046
C (19)	0.060	0.069
O (20)	0.099	0.094
C (21)	0.045	0.051
C (22)	0.043	0.049
H (23)	0.023	0.024
H (24)	0.008	0.008
H (25)	0.011	0.007
H (26)	0.006	0.007
H (27)	0.016	0.010
H (28)	0.019	0.013
H (29)	0.037	0.023
H (30)	0.022	0.022
H (31)	0.031	0.029
H (32)	0.041	0.027
H (33)	0.039	0.025

Table S4

Isorhamnetin(neutral)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.090	0.078
C (2)	0.035	0.045
C (3)	0.109	0.096
C (4)	0.007	0.024
C (5)	0.051	0.040
C (6)	0.029	0.033
C (7)	0.032	0.039
C (8)	0.033	0.032
C (9)	0.023	0.025
O (10)	0.040	0.044
O (11)	0.124	0.122
C (12)	0.001	0.020
C (13)	0.036	0.028
C (14)	0.013	0.018
C (15)	0.034	0.035
C (16)	0.017	0.022
C (17)	0.026	0.030
O (18)	0.013	0.007
C (19)	-0.007	0.004
O (20)	0.025	0.028
O (21)	0.029	0.030
O (22)	0.028	0.031
O (23)	0.031	0.031
H (24)	0.026	0.017
H (25)	0.028	0.018
H (26)	0.020	0.013
H (27)	0.020	0.012
H (28)	0.026	0.017
H (29)	0.007	0.003
H (30)	0.005	0.004
H (31)	0.005	0.003
H (32)	0.009	0.016
H (33)	0.010	0.012

H (34)	0.012	0.014
H (35)	0.013	0.012

Mulliken atomic charges:

	charge	spin
C (1)	0.266	0.000
C (2)	0.219	0.000
C (3)	0.315	0.000
C (4)	-0.059	0.000
C (5)	0.317	0.000
C (6)	-0.171	0.000
C (7)	0.355	0.000
C (8)	-0.177	0.000
C (9)	0.329	0.000
O (10)	-0.496	0.000
O (11)	-0.580	0.000
C (12)	0.016	0.000
C (13)	-0.132	0.000
C (14)	0.326	0.000
C (15)	0.296	0.000
C (16)	-0.087	0.000
C (17)	-0.098	0.000
O (18)	-0.562	0.000
C (19)	0.189	0.000
O (20)	-0.490	0.000
O (21)	-0.479	0.000
O (22)	-0.468	0.000
O (23)	-0.504	0.000
H (24)	0.061	0.000
H (25)	0.052	0.000
H (26)	0.058	0.000
H (27)	0.048	0.000
H (28)	0.048	0.000
H (29)	0.055	0.000
H (30)	0.055	0.000
H (31)	0.057	0.000
H (32)	0.297	0.000
H (33)	0.290	0.000
H (34)	0.286	0.000
H (35)	0.269	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.055	0.051
C (2)	0.069	0.073
C (3)	0.025	0.026
C (4)	0.014	0.017
C (5)	0.023	0.023
C (6)	0.023	0.023
C (7)	0.016	0.023
C (8)	0.041	0.040
C (9)	0.009	0.015
O (10)	0.030	0.038
O (11)	0.055	0.054
C (12)	0.022	0.035
C (13)	0.024	0.025
C (14)	0.031	0.032
C (15)	0.046	0.048
C (16)	0.026	0.034
C (17)	0.032	0.040
O (18)	0.024	0.035
C (19)	-0.006	0.010
O (20)	0.057	0.054
O (21)	0.021	0.022
O (22)	0.022	0.025
O (23)	0.088	0.086
H (24)	0.020	0.012
H (25)	0.028	0.017
H (26)	0.029	0.016

H (27)	0.032	0.021
H (28)	0.033	0.018
H (29)	0.013	0.009
H (30)	0.015	0.008
H (31)	0.012	0.008
H (32)	0.017	0.012
H (33)	0.009	0.009
H (34)	0.014	0.012
H (35)	0.031	0.031

Isorhamnetin(protonated)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.096	0.075
C (2)	0.034	0.048
C (3)	0.126	0.112
C (4)	0.001	0.025
C (5)	0.047	0.037
C (6)	0.024	0.028
C (7)	0.039	0.045
C (8)	0.031	0.031
C (9)	0.045	0.035
O (10)	0.011	0.026
O (11)	0.136	0.137
C (12)	-0.010	0.012
C (13)	0.025	0.020
C (14)	0.012	0.013
C (15)	0.026	0.026
C (16)	0.012	0.018
C (17)	0.024	0.024
O (18)	0.007	0.010
C (19)	-0.004	0.003
O (20)	0.022	0.022
O (21)	0.036	0.037
O (22)	0.027	0.031
O (23)	0.034	0.033
H (24)	0.026	0.016
H (25)	0.027	0.018
H (26)	0.025	0.021
H (27)	0.018	0.010
H (28)	0.017	0.011
H (29)	0.021	0.013
H (30)	0.005	0.003
H (31)	0.006	0.003
H (32)	0.005	0.003
H (33)	0.008	0.008
H (34)	0.013	0.014
H (35)	0.015	0.015

Mulliken atomic charges:

	charge	spin
C (1)	0.250	0.000
C (2)	0.270	0.000
C (3)	0.338	0.000
C (4)	-0.031	0.000
C (5)	0.337	0.000
C (6)	-0.144	0.000
C (7)	0.366	0.000
C (8)	-0.151	0.000
C (9)	0.345	0.000
O (10)	-0.432	0.000
O (11)	-0.500	0.000
C (12)	-0.010	0.000
C (13)	-0.123	0.000

C (14)	0.334	0.000
C (15)	0.311	0.000
C (16)	-0.076	0.000
C (17)	-0.069	0.000
O (18)	-0.555	0.000
C (19)	0.186	0.000
O (20)	-0.472	0.000
O (21)	-0.451	0.000
O (22)	-0.444	0.000
O (23)	-0.465	0.000
H (24)	0.080	0.000
H (25)	0.092	0.000
H (26)	0.367	0.000
H (27)	0.070	0.000
H (28)	0.058	0.000
H (29)	0.056	0.000
H (30)	0.060	0.000
H (31)	0.058	0.000
H (32)	0.061	0.000
H (33)	0.303	0.000
H (34)	0.300	0.000
H (35)	0.296	0.000
H (36)	0.283	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.029	0.023
C (2)	0.044	0.042
C (3)	0.013	0.014
C (4)	0.008	0.009
C (5)	0.010	0.009
C (6)	0.009	0.008
C (7)	0.008	0.010
C (8)	0.011	0.011
C (9)	0.001	0.005
O (10)	-0.002	0.009
O (11)	0.032	0.030
C (12)	0.041	0.061
C (13)	0.045	0.042
C (14)	0.060	0.065
C (15)	0.063	0.073
C (16)	0.045	0.051
C (17)	0.052	0.063
O (18)	0.079	0.079
C (19)	-0.016	0.021
O (20)	0.098	0.093
O (21)	0.010	0.011
O (22)	0.009	0.010
O (23)	0.048	0.048
H (24)	0.008	0.005
H (25)	0.011	0.006
H (26)	0.011	0.007
H (27)	0.040	0.024
H (28)	0.044	0.028
H (29)	0.046	0.029
H (30)	0.032	0.020
H (31)	0.031	0.019
H (32)	0.024	0.015
H (33)	0.028	0.031
H (34)	0.004	0.004
H (35)	0.004	0.005
H (36)	0.021	0.020

TableS5

ASCROBIC ACID (NEUTRAL)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
O (1)	0.062	0.069
C (2)	-0.030	0.027
C (3)	0.166	0.130
C (4)	0.065	0.081
C (5)	0.176	0.156
O (6)	0.181	0.183
O (7)	0.053	0.055
O (8)	0.075	0.083
C (9)	-0.006	0.015
C (10)	-0.006	0.008
O (11)	0.011	0.011
O (12)	0.026	0.023
H (13)	0.084	0.049
H (14)	0.022	0.023
H (15)	0.031	0.033
H (16)	0.032	0.015
H (17)	0.019	0.013
H (18)	0.018	0.009
H (19)	0.009	0.006
H (20)	0.009	0.011

Mulliken atomic charges:

atom	charge	spin
O (1)	-0.542	0.000
C (2)	0.195	0.000
C (3)	0.260	0.000
C (4)	0.215	0.000
C (5)	0.536	0.000
O (6)	-0.524	0.000
O (7)	-0.500	0.000
O (8)	-0.466	0.000
C (9)	0.217	0.000
C (10)	0.234	0.000
O (11)	-0.561	0.000
O (12)	-0.530	0.000
H (13)	0.079	0.000
H (14)	0.294	0.000
H (15)	0.303	0.000
H (16)	0.041	0.000
H (17)	0.048	0.000
H (18)	0.034	0.000
H (19)	0.282	0.000
H (20)	0.284	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
O (1)	0.043	0.042
C (2)	-0.019	0.021
C (3)	0.122	0.117
C (4)	0.133	0.138
C (5)	0.054	0.051
O (6)	0.103	0.099
O (7)	0.178	0.168
O (8)	0.122	0.119
C (9)	-0.005	0.012
C (10)	-0.002	0.009
O (11)	0.017	0.017
O (12)	0.028	0.025
H (13)	0.058	0.034
H (14)	0.049	0.057

H (15)	0.038	0.043
H (16)	0.029	0.014
H (17)	0.018	0.010
H (18)	0.014	0.008
H (19)	0.007	0.008
H (20)	0.012	0.010

ASCROBIC ACID (PROTONATED)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
o (1)	0.076	0.082
c (2)	-0.015	0.030
c (3)	0.143	0.126
c (4)	0.054	0.066
c (5)	0.170	0.151
o (6)	0.106	0.110
o (7)	0.080	0.063
o (8)	0.094	0.098
c (9)	0.000	0.019
c (10)	-0.012	0.010
o (11)	0.016	0.017
o (12)	0.028	0.023
H (13)	0.081	0.050
H (14)	0.035	0.038
H (15)	0.013	0.021
H (16)	0.030	0.040
H (17)	0.040	0.019
H (18)	0.020	0.015
H (19)	0.020	0.012
H (20)	0.010	0.003
H (21)	0.012	0.011

Mulliken atomic charges:
charge spin

o (1)	-0.445	0.000
c (2)	0.181	0.000
c (3)	0.322	0.000
c (4)	0.251	0.000
c (5)	0.621	0.000

O (6)	-0.368	0.000
O (7)	-0.513	0.000
O (8)	-0.395	0.000
C (9)	0.217	0.000
C (10)	0.229	0.000
O (11)	-0.544	0.000
O (12)	-0.509	0.000
H (13)	0.125	0.000
H (14)	0.334	0.000
H (15)	0.321	0.000
H (16)	0.321	0.000
H (17)	0.065	0.000
H (18)	0.058	0.000
H (19)	0.048	0.000
H (20)	0.285	0.000
H (21)	0.295	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
O (1)	0.011	0.010
C (2)	-0.007	0.014
C (3)	0.046	0.025
C (4)	0.026	0.029
C (5)	0.026	0.020
O (6)	0.026	0.026
O (7)	-0.014	0.004
O (8)	0.019	0.022
C (9)	-0.018	0.042
C (10)	-0.016	0.061
O (11)	0.341	0.303
O (12)	0.142	0.128
H (13)	0.035	0.019
H (14)	0.007	0.010
H (15)	0.020	0.013
H (16)	0.015	0.008
H (17)	0.060	0.031
H (18)	0.085	0.048
H (19)	0.093	0.057
H (20)	0.066	0.085
H (21)	0.038	0.043

Table S6

Erucic acid (neutral)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.287	0.254
C (2)	-0.038	0.046
C (3)	-0.022	0.027
C (4)	-0.014	0.005
C (5)	-0.003	0.005
C (6)	-0.004	0.002
C (7)	0.001	0.001
C (8)	-0.003	0.000
C (9)	0.002	0.001
C (10)	0.001	0.000
C (11)	-0.002	-0.001
C (12)	0.001	0.000
C (13)	-0.005	0.001
C (14)	0.004	0.000
C (15)	0.002	-0.001
C (16)	0.000	0.000
C (17)	-0.001	-0.001
C (18)	-0.001	0.000

C (19)	-0.003	0.000
C (20)	-0.001	0.000
C (21)	-0.002	-0.001
C (22)	0.000	0.000
O (23)	0.255	0.262
O (24)	0.129	0.138
H (25)	0.106	0.066
H (26)	0.072	0.038
H (27)	0.034	0.021
H (28)	0.059	0.033
H (29)	0.023	0.011
H (30)	0.013	0.009
H (31)	0.010	0.006
H (32)	0.011	0.005
H (33)	0.005	0.003
H (34)	0.005	0.003
H (35)	0.003	0.002
H (36)	0.002	0.001
H (37)	0.003	0.003
H (38)	0.000	-0.002
H (39)	0.000	0.002
H (40)	-0.001	-0.002
H (41)	0.002	0.002
H (42)	0.000	-0.001
H (43)	-0.002	0.000
H (44)	-0.002	-0.003
H (45)	-0.001	0.000
H (46)	-0.001	-0.003
H (47)	0.001	0.002
H (48)	0.002	0.001
H (49)	0.000	0.001
H (50)	0.000	0.000
H (51)	0.000	0.000
H (52)	0.002	0.001
H (53)	-0.002	0.000
H (54)	0.000	0.000
H (55)	0.002	0.000
H (56)	0.001	0.000
H (57)	-0.001	0.001
H (58)	0.003	0.000
H (59)	0.000	-0.002
H (60)	0.001	0.001
H (61)	-0.002	-0.001
H (62)	0.002	0.000
H (63)	0.001	0.001
H (64)	0.000	0.000
H (65)	0.000	0.001
H (66)	0.065	0.061

Mulliken atomic charges:
charge spin

C (1)	0.528	0.000
C (2)	-0.092	0.000
C (3)	-0.037	0.000
C (4)	-0.032	0.000
C (5)	-0.030	0.000
C (6)	-0.032	0.000
C (7)	-0.033	0.000
C (8)	-0.032	0.000
C (9)	-0.034	0.000
C (10)	-0.035	0.000
C (11)	-0.028	0.000
C (12)	-0.038	0.000
C (13)	-0.035	0.000
C (14)	-0.034	0.000
C (15)	-0.041	0.000
C (16)	-0.024	0.000
C (17)	-0.033	0.000
C (18)	-0.031	0.000
C (19)	-0.029	0.000
C (20)	-0.026	0.000

C (21)	-0.031	0.000
C (22)	-0.065	0.000
O (23)	-0.524	0.000
O (24)	-0.450	0.000
H (25)	0.056	0.000
H (26)	0.047	0.000
H (27)	0.035	0.000
H (28)	0.029	0.000
H (29)	0.021	0.000
H (30)	0.025	0.000
H (31)	0.019	0.000
H (32)	0.018	0.000
H (33)	0.016	0.000
H (34)	0.020	0.000
H (35)	0.018	0.000
H (36)	0.014	0.000
H (37)	0.015	0.000
H (38)	0.019	0.000
H (39)	0.018	0.000
H (40)	0.015	0.000
H (41)	0.017	0.000
H (42)	0.021	0.000
H (43)	0.019	0.000
H (44)	0.018	0.000
H (45)	0.020	0.000
H (46)	0.037	0.000
H (47)	0.003	0.000
H (48)	0.003	0.000
H (49)	0.034	0.000
H (50)	0.019	0.000
H (51)	0.018	0.000
H (52)	0.019	0.000
H (53)	0.019	0.000
H (54)	0.017	0.000
H (55)	0.015	0.000
H (56)	0.017	0.000
H (57)	0.016	0.000
H (58)	0.015	0.000
H (59)	0.014	0.000
H (60)	0.015	0.000
H (61)	0.017	0.000
H (62)	0.016	0.000
H (63)	0.020	0.000
H (64)	0.020	0.000
H (65)	0.018	0.000
H (66)	0.283	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	-0.001	0.000
C (2)	-0.002	-0.001
C (3)	-0.001	-0.001
C (4)	-0.002	0.000
C (5)	0.000	0.000
C (6)	0.002	0.001
C (7)	-0.002	0.001
C (8)	0.001	0.002
C (9)	-0.005	0.004
C (10)	-0.007	0.006
C (11)	-0.006	0.019
C (12)	-0.033	0.038
C (13)	0.180	0.206
C (14)	0.167	0.206
C (15)	-0.034	0.038
C (16)	-0.009	0.019
C (17)	-0.004	0.008
C (18)	-0.002	0.004
C (19)	0.002	0.003
C (20)	0.000	0.001

C (21)	0.002	0.001
C (22)	0.000	0.000
O (23)	0.003	0.001
O (24)	0.001	0.004
H (25)	0.001	0.002
H (26)	0.000	0.000
H (27)	0.004	-0.002
H (28)	-0.002	0.000
H (29)	0.000	-0.001
H (30)	0.001	0.000
H (31)	0.000	-0.001
H (32)	0.000	0.001
H (33)	0.000	0.000
H (34)	0.000	0.000
H (35)	0.001	0.000
H (36)	0.002	0.001
H (37)	0.002	-0.001
H (38)	0.004	0.004
H (39)	0.006	0.001
H (40)	0.008	0.006
H (41)	0.012	0.005
H (42)	0.014	0.009
H (43)	0.029	0.014
H (44)	0.037	0.021
H (45)	0.060	0.032
H (46)	0.090	0.062
H (47)	0.111	0.067
H (48)	0.111	0.069
H (49)	0.087	0.057
H (50)	0.057	0.030
H (51)	0.036	0.019
H (52)	0.028	0.014
H (53)	0.016	0.008
H (54)	0.014	0.007
H (55)	0.005	0.004
H (56)	0.007	0.004
H (57)	0.005	0.001
H (58)	0.001	0.002
H (59)	0.002	0.003
H (60)	0.001	0.000
H (61)	0.003	0.001
H (62)	-0.001	0.000
H (63)	0.000	0.000
H (64)	0.000	0.000
H (65)	0.001	0.000
H (66)	0.001	0.001

ERUCIC ACID (PROTONATED)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.395	0.313
C (2)	-0.038	0.070
C (3)	-0.016	0.052
C (4)	-0.015	0.009
C (5)	-0.006	0.007
C (6)	-0.003	0.004
C (7)	-0.001	0.002
C (8)	0.000	0.001
C (9)	0.000	0.001
C (10)	0.000	0.001
C (11)	0.000	0.000
C (12)	0.000	0.000
C (13)	0.000	0.000
C (14)	0.001	0.000
C (15)	0.000	0.000

C (16)	0.000	0.000
C (17)	0.000	0.000
C (18)	0.000	0.000
C (19)	0.000	0.000
C (20)	0.000	0.000
C (21)	0.000	0.000
C (22)	0.000	0.000
O (23)	0.253	0.280
O (24)	0.000	0.000
H (25)	0.092	0.062
H (26)	0.101	0.069
H (27)	0.074	0.044
H (28)	0.059	0.032
H (29)	0.027	0.014
H (30)	0.028	0.013
H (31)	0.013	0.007
H (32)	0.013	0.007
H (33)	0.007	0.003
H (34)	0.006	0.003
H (35)	0.003	0.001
H (36)	0.003	0.001
H (37)	0.001	0.001
H (38)	0.001	0.001
H (39)	0.001	0.000
H (40)	0.001	0.000
H (41)	0.000	0.000
H (42)	0.000	0.000
H (43)	0.000	0.000
H (44)	0.000	0.000
H (45)	0.000	0.000
H (46)	0.000	0.000
H (47)	0.000	0.000
H (48)	0.000	0.000
H (49)	-0.001	0.000
H (50)	0.000	0.000
H (51)	0.000	0.000
H (52)	0.000	0.000
H (53)	0.000	0.000
H (54)	0.000	0.000
H (55)	0.000	0.000
H (56)	0.000	0.000
H (57)	0.000	0.000
H (58)	0.000	0.000
H (59)	0.000	0.000
H (60)	-0.001	0.000
H (61)	0.000	0.000
H (62)	0.000	0.000
H (63)	0.000	0.000
H (64)	0.000	0.000
H (65)	0.000	0.000
H (66)	0.000	0.000
H (67)	0.000	0.000

Mulliken atomic charges:
charge spin

C (1)	0.579	0.000
C (2)	-0.149	0.000
C (3)	-0.041	0.000
C (4)	-0.043	0.000
C (5)	-0.033	0.000
C (6)	-0.034	0.000
C (7)	-0.032	0.000
C (8)	-0.032	0.000
C (9)	-0.031	0.000
C (10)	-0.033	0.000
C (11)	-0.015	0.000
C (12)	-0.045	0.000

C (13)	-0.030	0.000
C (14)	-0.033	0.000
C (15)	-0.043	0.000
C (16)	-0.014	0.000
C (17)	-0.032	0.000
C (18)	-0.030	0.000
C (19)	-0.029	0.000
C (20)	-0.025	0.000
C (21)	-0.030	0.000
C (22)	-0.065	0.000
O (23)	-0.082	0.000
O (24)	-0.555	0.000
H (25)	0.170	0.000
H (26)	0.173	0.000
H (27)	0.081	0.000
H (28)	0.078	0.000
H (29)	0.044	0.000
H (30)	0.045	0.000
H (31)	0.031	0.000
H (32)	0.029	0.000
H (33)	0.021	0.000
H (34)	0.022	0.000
H (35)	0.019	0.000
H (36)	0.018	0.000
H (37)	0.016	0.000
H (38)	0.017	0.000
H (39)	0.018	0.000
H (40)	0.016	0.000
H (41)	0.017	0.000
H (42)	0.018	0.000
H (43)	0.018	0.000
H (44)	0.017	0.000
H (45)	0.017	0.000
H (46)	0.030	0.000
H (47)	0.004	0.000
H (48)	0.003	0.000
H (49)	0.030	0.000
H (50)	0.017	0.000
H (51)	0.016	0.000
H (52)	0.017	0.000
H (53)	0.018	0.000
H (54)	0.017	0.000
H (55)	0.016	0.000
H (56)	0.016	0.000
H (57)	0.016	0.000
H (58)	0.016	0.000
H (59)	0.014	0.000
H (60)	0.015	0.000
H (61)	0.016	0.000
H (62)	0.016	0.000
H (63)	0.020	0.000
H (64)	0.020	0.000
H (65)	0.018	0.000
H (66)	0.277	0.000
H (67)	0.278	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.001	0.001
C (2)	-0.002	0.000
C (3)	0.001	0.000
C (4)	0.001	0.000
C (5)	-0.001	0.001
C (6)	0.000	0.001
C (7)	-0.001	0.002
C (8)	-0.002	0.003
C (9)	-0.004	0.005
C (10)	-0.004	0.009
C (11)	-0.010	0.023

C (12)	-0.030	0.035
C (13)	0.166	0.201
C (14)	0.165	0.201
C (15)	-0.030	0.035
C (16)	-0.010	0.024
C (17)	-0.005	0.010
C (18)	-0.003	0.006
C (19)	-0.002	0.003
C (20)	-0.001	0.002
C (21)	0.000	0.001
C (22)	0.000	0.001
O (23)	-0.001	0.000
O (24)	0.000	0.000
H (25)	0.004	0.002
H (26)	0.000	0.000
H (27)	-0.001	0.000
H (28)	-0.001	-0.001
H (29)	-0.003	-0.001
H (30)	0.000	0.000
H (31)	0.002	0.001
H (32)	0.001	0.000
H (33)	0.001	0.001
H (34)	0.002	0.001
H (35)	0.003	0.002
H (36)	0.003	0.001
H (37)	0.005	0.002
H (38)	0.005	0.002
H (39)	0.008	0.005
H (40)	0.009	0.005
H (41)	0.016	0.008
H (42)	0.015	0.008
H (43)	0.033	0.017
H (44)	0.038	0.019
H (45)	0.054	0.028
H (46)	0.080	0.051
H (47)	0.112	0.068
H (48)	0.112	0.069
H (49)	0.081	0.051
H (50)	0.053	0.028
H (51)	0.039	0.019
H (52)	0.034	0.017
H (53)	0.016	0.008
H (54)	0.016	0.008
H (55)	0.009	0.005
H (56)	0.009	0.004
H (57)	0.005	0.002
H (58)	0.004	0.002
H (59)	0.002	0.001
H (60)	0.003	0.001
H (61)	0.001	0.001
H (62)	0.001	0.001
H (63)	0.001	0.000
H (64)	0.001	0.000
H (65)	0.001	0.001
H (66)	0.000	0.000
H (67)	0.000	0.000

TableS7

OLEIC ACID(NEUTRAL)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.292	0.263
C (2)	-0.046	0.046
C (3)	-0.027	0.010
C (4)	-0.014	0.004
C (5)	-0.001	0.003

C (6)	0.002	0.002
C (7)	-0.003	0.001
C (8)	-0.005	0.001
C (9)	-0.001	0.000
C (10)	0.009	0.001
C (11)	-0.006	0.000
C (12)	0.000	-0.002
C (13)	0.002	0.000
C (14)	0.002	0.000
C (15)	-0.001	0.000
C (16)	0.002	0.000
C (17)	0.002	0.000
C (18)	0.002	0.000
O (19)	0.249	0.253
O (20)	0.144	0.155
H (21)	0.085	0.046
H (22)	0.127	0.085
H (23)	0.036	0.021
H (24)	0.035	0.018
H (25)	0.014	0.008
H (26)	0.022	0.011
H (27)	0.004	0.004
H (28)	0.008	0.005
H (29)	0.004	0.000
H (30)	0.005	0.002
H (31)	0.000	0.001
H (32)	0.002	0.002
H (33)	0.001	0.000
H (34)	0.002	-0.001
H (35)	0.000	-0.001
H (36)	0.000	-0.001
H (37)	0.003	0.004
H (38)	-0.002	-0.002
H (39)	-0.001	0.002
H (40)	-0.006	-0.005
H (41)	0.003	0.001
H (42)	-0.002	0.000
H (43)	-0.001	0.000
H (44)	0.000	0.000
H (45)	0.000	-0.001
H (46)	0.000	0.001
H (47)	-0.002	0.000
H (48)	0.002	0.002
H (49)	-0.001	0.000
H (50)	-0.001	0.000
H (51)	-0.001	0.000
H (52)	0.000	0.001
H (53)	-0.001	-0.001
H (54)	0.062	0.061

Mulliken atomic charges:
charge spin

C (1)	0.539	0.000
C (2)	-0.107	0.000
C (3)	-0.023	0.000
C (4)	-0.033	0.000
C (5)	-0.031	0.000
C (6)	-0.034	0.000
C (7)	-0.019	0.000
C (8)	-0.081	0.000
C (9)	-0.023	0.000
C (10)	-0.022	0.000
C (11)	-0.080	0.000
C (12)	-0.021	0.000
C (13)	-0.034	0.000
C (14)	-0.030	0.000
C (15)	-0.031	0.000
C (16)	-0.026	0.000
C (17)	-0.032	0.000
C (18)	-0.065	0.000

O (19)	-0.524	0.000
O (20)	-0.453	0.000
H (21)	0.054	0.000
H (22)	0.062	0.000
H (23)	0.029	0.000
H (24)	0.027	0.000
H (25)	0.023	0.000
H (26)	0.020	0.000
H (27)	0.021	0.000
H (28)	0.018	0.000
H (29)	0.017	0.000
H (30)	0.020	0.000
H (31)	0.021	0.000
H (32)	0.020	0.000
H (33)	0.026	0.000
H (34)	0.034	0.000
H (35)	0.018	0.000
H (36)	0.018	0.000
H (37)	0.035	0.000
H (38)	0.026	0.000
H (39)	0.020	0.000
H (40)	0.020	0.000
H (41)	0.019	0.000
H (42)	0.016	0.000
H (43)	0.016	0.000
H (44)	0.018	0.000
H (45)	0.017	0.000
H (46)	0.015	0.000
H (47)	0.015	0.000
H (48)	0.016	0.000
H (49)	0.017	0.000
H (50)	0.016	0.000
H (51)	0.020	0.000
H (52)	0.020	0.000
H (53)	0.018	0.000
H (54)	0.281	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.009	0.000
C (2)	-0.006	0.004
C (3)	0.006	0.004
C (4)	0.003	0.002
C (5)	-0.005	0.005
C (6)	-0.007	0.008
C (7)	-0.011	0.020
C (8)	-0.020	0.035
C (9)	0.172	0.209
C (10)	0.165	0.209
C (11)	-0.019	0.036
C (12)	-0.012	0.021
C (13)	-0.006	0.008
C (14)	-0.005	0.004
C (15)	-0.001	0.003
C (16)	-0.002	0.001
C (17)	-0.002	0.001
C (18)	-0.002	0.001
O (19)	0.003	0.004
O (20)	-0.013	-0.009
H (21)	0.003	0.006
H (22)	0.002	-0.002
H (23)	0.003	0.002
H (24)	0.000	-0.001
H (25)	0.002	0.002
H (26)	-0.002	-0.001
H (27)	0.010	0.004
H (28)	0.007	0.002
H (29)	0.015	0.009
H (30)	0.012	0.007
H (31)	0.032	0.015
H (32)	0.037	0.017
H (33)	0.052	0.026

H (34)	0.081	0.055
H (35)	0.113	0.073
H (36)	0.114	0.074
H (37)	0.081	0.052
H (38)	0.055	0.029
H (39)	0.037	0.017
H (40)	0.035	0.020
H (41)	0.011	0.006
H (42)	0.016	0.007
H (43)	0.009	0.004
H (44)	0.007	0.003
H (45)	0.004	0.003
H (46)	0.004	0.000
H (47)	0.004	0.001
H (48)	0.000	-0.001
H (49)	0.002	0.000
H (50)	0.002	0.000
H (51)	0.002	0.000
H (52)	0.001	0.000
H (53)	0.002	0.001
H (54)	0.003	0.002

OLEIC ACID (PROTONATED)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.289	0.254
C (2)	-0.039	0.047
C (3)	-0.015	0.033
C (4)	-0.012	0.006
C (5)	-0.004	0.006
C (6)	-0.002	0.003
C (7)	-0.001	0.001
C (8)	0.001	0.001
C (9)	0.000	0.000
C (10)	0.001	0.001
C (11)	0.000	0.000
C (12)	0.000	0.000
C (13)	0.000	0.000
C (14)	0.000	0.000
C (15)	0.000	0.000
C (16)	0.000	0.000
C (17)	0.000	0.000
C (18)	0.000	0.000
O (19)	0.161	0.165
O (20)	0.163	0.163
H (21)	0.073	0.041
H (22)	0.096	0.061
H (23)	0.056	0.033
H (24)	0.043	0.022
H (25)	0.015	0.007
H (26)	0.023	0.011
H (27)	0.010	0.005
H (28)	0.010	0.005
H (29)	0.004	0.002
H (30)	0.004	0.002
H (31)	0.002	0.001
H (32)	0.001	0.000
H (33)	0.001	0.001
H (34)	0.000	0.000
H (35)	0.000	0.000
H (36)	0.001	0.001
H (37)	0.000	-0.001
H (38)	0.001	0.000
H (39)	0.000	0.000
H (40)	0.000	0.000
H (41)	0.001	0.001
H (42)	0.000	0.000
H (43)	0.000	0.000

H (44)	0.000	0.000
H (45)	0.000	0.000
H (46)	0.000	0.000
H (47)	0.000	0.000
H (48)	0.000	0.000
H (49)	0.000	0.000
H (50)	0.000	0.000
H (51)	0.000	0.000
H (52)	0.000	0.000
H (53)	0.000	0.000
H (54)	0.057	0.063
H (55)	0.056	0.062

Mulliken atomic charges:

	charge	spin
C (1)	0.632	0.000
C (2)	-0.111	0.000
C (3)	-0.043	0.000
C (4)	-0.034	0.000
C (5)	-0.032	0.000
C (6)	-0.035	0.000
C (7)	-0.020	0.000
C (8)	-0.079	0.000
C (9)	-0.025	0.000
C (10)	-0.022	0.000
C (11)	-0.076	0.000
C (12)	-0.022	0.000
C (13)	-0.034	0.000
C (14)	-0.031	0.000
C (15)	-0.030	0.000
C (16)	-0.025	0.000
C (17)	-0.031	0.000
C (18)	-0.065	0.000
O (19)	-0.309	0.000
O (20)	-0.314	0.000
H (21)	0.093	0.000
H (22)	0.105	0.000
H (23)	0.055	0.000
H (24)	0.054	0.000
H (25)	0.033	0.000
H (26)	0.032	0.000
H (27)	0.025	0.000
H (28)	0.025	0.000
H (29)	0.022	0.000
H (30)	0.021	0.000
H (31)	0.021	0.000
H (32)	0.019	0.000
H (33)	0.036	0.000
H (34)	0.027	0.000
H (35)	0.016	0.000
H (36)	0.016	0.000
H (37)	0.035	0.000
H (38)	0.029	0.000
H (39)	0.020	0.000
H (40)	0.020	0.000
H (41)	0.018	0.000
H (42)	0.017	0.000
H (43)	0.016	0.000
H (44)	0.018	0.000
H (45)	0.016	0.000
H (46)	0.015	0.000
H (47)	0.014	0.000
H (48)	0.016	0.000
H (49)	0.016	0.000
H (50)	0.016	0.000
H (51)	0.020	0.000
H (52)	0.020	0.000
H (53)	0.018	0.000
H (54)	0.340	0.000
H (55)	0.341	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	-0.001	0.000
C (2)	0.000	0.000
C (3)	-0.001	0.001
C (4)	-0.001	0.002
C (5)	-0.004	0.004
C (6)	-0.005	0.008
C (7)	-0.009	0.021
C (8)	-0.030	0.035
C (9)	0.175	0.210
C (10)	0.176	0.210
C (11)	-0.029	0.036
C (12)	-0.011	0.018
C (13)	-0.005	0.007
C (14)	-0.003	0.004
C (15)	-0.001	0.003
C (16)	-0.001	0.001
C (17)	0.000	0.001
C (18)	0.000	0.000
O (19)	0.002	0.001
O (20)	0.002	0.001
H (21)	0.000	0.000
H (22)	0.001	0.000
H (23)	0.003	0.002
H (24)	0.001	0.000
H (25)	0.004	0.003
H (26)	0.003	0.002
H (27)	0.008	0.004
H (28)	0.007	0.004
H (29)	0.015	0.008
H (30)	0.015	0.008
H (31)	0.037	0.019
H (32)	0.031	0.017
H (33)	0.082	0.053
H (34)	0.052	0.026
H (35)	0.115	0.073
H (36)	0.113	0.072
H (37)	0.087	0.058
H (38)	0.053	0.027
H (39)	0.036	0.018
H (40)	0.028	0.014
H (41)	0.013	0.007
H (42)	0.014	0.007
H (43)	0.007	0.003
H (44)	0.007	0.004
H (45)	0.003	0.002
H (46)	0.004	0.002
H (47)	0.002	0.001
H (48)	0.002	0.001
H (49)	0.001	0.001
H (50)	0.001	0.000
H (51)	0.001	0.000
H (52)	0.000	0.000
H (53)	0.001	0.001
H (54)	-0.001	0.000
H (55)	-0.001	0.000

Table S8
GALLIC ACID(NEUTRAL)

Fukui Indices for Nucleophilic Attack (Fukui(+))		
atom	Mulliken	Hirshfeld
C (1)	0.147	0.133
C (2)	0.023	0.064
C (3)	0.084	0.076
C (4)	0.026	0.041

O (5)	0.030	0.032
C (6)	0.093	0.077
O (7)	0.048	0.054
C (8)	0.026	0.040
O (9)	0.026	0.029
C (10)	0.084	0.073
O (11)	0.147	0.145
O (12)	0.068	0.078
H (13)	0.055	0.037
H (14)	0.014	0.014
H (15)	0.020	0.021
H (16)	0.014	0.015
H (17)	0.056	0.036
H (18)	0.039	0.036

Mulliken atomic charges:
charge spin

C (1)	0.526	0.000
C (2)	0.005	0.000
C (3)	-0.134	0.000
C (4)	0.306	0.000
O (5)	-0.498	0.000
C (6)	0.244	0.000
O (7)	-0.496	0.000
C (8)	0.303	0.000
O (9)	-0.504	0.000
C (10)	-0.142	0.000
O (11)	-0.530	0.000
O (12)	-0.458	0.000
H (13)	0.054	0.000
H (14)	0.295	0.000
H (15)	0.303	0.000
H (16)	0.293	0.000
H (17)	0.052	0.000
H (18)	0.283	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.036	0.031
C (2)	0.058	0.083
C (3)	0.048	0.047
C (4)	0.070	0.083
O (5)	0.114	0.108
C (6)	0.100	0.104
O (7)	0.128	0.122
C (8)	0.050	0.054
O (9)	0.050	0.052
C (10)	0.059	0.060
O (11)	0.056	0.056
O (12)	0.022	0.026
H (13)	0.050	0.029
H (14)	0.032	0.036
H (15)	0.037	0.041
H (16)	0.022	0.024
H (17)	0.049	0.031
H (18)	0.018	0.015

GALLIC ACID(PROTONATED)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.169	0.145
C (2)	-0.007	0.045
C (3)	0.091	0.076
C (4)	0.023	0.039
O (5)	0.029	0.031

C (6)	0.093	0.081
O (7)	0.056	0.063
C (8)	0.026	0.039
O (9)	0.026	0.028
C (10)	0.086	0.072
O (11)	0.088	0.093
O (12)	0.086	0.091
H (13)	0.055	0.036
H (14)	0.017	0.015
H (15)	0.025	0.025
H (16)	0.019	0.017
H (17)	0.049	0.032
H (18)	0.032	0.035
H (19)	0.037	0.037

Mulliken atomic charges:
charge spin

C (1)	0.615	0.000
C (2)	0.035	0.000
C (3)	-0.109	0.000
C (4)	0.323	0.000
O (5)	-0.478	0.000
C (6)	0.275	0.000
O (7)	-0.454	0.000
C (8)	0.315	0.000
O (9)	-0.484	0.000
C (10)	-0.135	0.000
O (11)	-0.381	0.000
O (12)	-0.362	0.000
H (13)	0.081	0.000
H (14)	0.303	0.000
H (15)	0.315	0.000
H (16)	0.303	0.000
H (17)	0.079	0.000
H (18)	0.323	0.000
H (19)	0.333	0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.055	0.050
C (2)	0.033	0.063
C (3)	0.066	0.062
C (4)	0.070	0.090
O (5)	0.156	0.144
C (6)	0.080	0.081
O (7)	0.109	0.101
C (8)	0.039	0.040
O (9)	0.039	0.040
C (10)	0.062	0.058
O (11)	0.051	0.047
O (12)	0.047	0.043
H (13)	0.048	0.031
H (14)	0.036	0.044
H (15)	0.028	0.032
H (16)	0.013	0.017
H (17)	0.042	0.027
H (18)	0.011	0.014
H (19)	0.014	0.018

Table S9

Kaempferol (Neutral)

Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.091	0.078
C (2)	0.035	0.046
C (3)	0.110	0.096
C (4)	0.006	0.024
C (5)	0.051	0.040
C (6)	0.028	0.033
C (7)	0.030	0.038
C (8)	0.034	0.032
C (9)	0.022	0.025
O (10)	0.039	0.044
O (11)	0.120	0.120
C (12)	-0.004	0.020
C (13)	0.033	0.032
C (14)	0.014	0.022
C (15)	0.035	0.035
C (16)	0.014	0.022
C (17)	0.034	0.030
O (18)	0.024	0.026
O (19)	0.028	0.030
O (20)	0.026	0.030
O (21)	0.031	0.030
H (22)	0.028	0.018
H (23)	0.029	0.018
H (24)	0.024	0.016
H (25)	0.021	0.013
H (26)	0.021	0.013
H (27)	0.024	0.015
H (28)	0.009	0.010
H (29)	0.011	0.012
H (30)	0.015	0.015
H (31)	0.016	0.016

ken atomic chargesMULKIN

	charge	spin
C (1)	0.273	0.000
C (2)	0.215	0.000
C (3)	0.316	0.000
C (4)	-0.059	0.000
C (5)	0.317	0.000
C (6)	-0.172	0.000
C (7)	0.354	0.000
C (8)	-0.177	0.000
C (9)	0.330	0.000
O (10)	-0.495	0.000
O (11)	-0.579	0.000
C (12)	0.013	0.000
C (13)	-0.040	0.000
C (14)	-0.086	0.000
C (15)	0.343	0.000
C (16)	-0.081	0.000
C (17)	-0.076	0.000
O (18)	-0.484	0.000
O (19)	-0.479	0.000
O (20)	-0.468	0.000
O (21)	-0.504	0.000
H (22)	0.061	0.000
H (23)	0.052	0.000

H (24)	0.045	0.000
H (25)	0.050	0.000
H (26)	0.046	0.000
H (27)	0.049	0.000
H (28)	0.288	0.000
H (29)	0.290	0.000
H (30)	0.285	0.000
H (31)	0.271	0.000

Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.065	0.061
C (2)	0.080	0.082
C (3)	0.027	0.029
C (4)	0.018	0.020
C (5)	0.030	0.031
C (6)	0.031	0.030
C (7)	0.020	0.029
C (8)	0.055	0.055
C (9)	0.012	0.018
O (10)	0.040	0.047
O (11)	0.064	0.061
C (12)	0.016	0.025
C (13)	0.026	0.027
C (14)	0.023	0.028
C (15)	0.027	0.035
C (16)	0.025	0.029
C (17)	0.011	0.023
O (18)	0.041	0.040
O (19)	0.028	0.028
O (20)	0.034	0.036
O (21)	0.100	0.097
H (22)	0.024	0.015
H (23)	0.035	0.022
H (24)	0.027	0.015
H (25)	0.023	0.015
H (26)	0.024	0.016
H (27)	0.027	0.015
H (28)	0.013	0.014
H (29)	0.011	0.012
H (30)	0.014	0.015
H (31)	0.029	0.029

Kaempferol(protonated)

Fukui Indices for Nucleophilic Attack (Fukui(+))

atom	Mulliken	Hirshfeld
C (1)	0.103	0.076
C (2)	0.031	0.049
C (3)	0.127	0.113
C (4)	0.002	0.025
C (5)	0.048	0.038
C (6)	0.024	0.029
C (7)	0.040	0.046
C (8)	0.029	0.031
C (9)	0.042	0.033
O (10)	0.009	0.025
O (11)	0.137	0.138
C (12)	-0.007	0.012
C (13)	0.022	0.024
C (14)	0.013	0.018
C (15)	0.023	0.025
C (16)	0.013	0.018
C (17)	0.020	0.023
O (18)	0.021	0.022
O (19)	0.035	0.037
O (20)	0.028	0.032

O (21)	0.034	0.034
H (22)	0.027	0.017
H (23)	0.028	0.018
H (24)	0.020	0.017
H (25)	0.021	0.012
H (26)	0.017	0.011
H (27)	0.017	0.011
H (28)	0.021	0.012
H (29)	0.008	0.008
H (30)	0.015	0.015
H (31)	0.015	0.015
H (32)	0.017	0.017

Mulliken atomic charges:
charge spin

C (1)	0.257	0.000
C (2)	0.268	0.000
C (3)	0.339	0.000
C (4)	-0.033	0.000
C (5)	0.335	0.000
C (6)	-0.146	0.000
C (7)	0.365	0.000
C (8)	-0.151	0.000
C (9)	0.349	0.000
O (10)	-0.430	0.000
O (11)	-0.500	0.000
C (12)	-0.016	0.000
C (13)	-0.031	0.000
C (14)	-0.076	0.000
C (15)	0.357	0.000
C (16)	-0.069	0.000
C (17)	-0.045	0.000
O (18)	-0.466	0.000
O (19)	-0.451	0.000
O (20)	-0.444	0.000
O (21)	-0.466	0.000
H (22)	0.081	0.000
H (23)	0.091	0.000
H (24)		
H (25)	0.059	0.000
H (26)	0.367	0.000
0.061		

0.000
 H (27)
 0.057
 0.000
 H (28)
 0.058
 0.000
 H (29)
 0.294
 0.000
 H (30)
 0.301
 0.000
 H (31)
 0.296
 0.000
 H (32)
 0.286
 0.000

Fukui Indices for Electrophilic Attack (Fukui(-))

atom	Mulliken	Hirshfeld
C (1)	0.044	0.045
C (2)	0.063	0.060
C (3)	0.016	0.018
C (4)	0.018	0.019
C (5)	0.017	0.018
C (6)	0.015	0.014
C (7)	0.011	0.017
C (8)	0.031	0.029
C (9)	0.008	0.012
O (10)	0.004	0.016
O (11)	0.041	0.039
C (12)	0.043	0.062
C (13)	0.037	0.041
C (14)	0.050	0.053
C (15)	0.043	0.061
C (16)	0.052	0.056
C (17)	0.029	0.037
O (18)	0.093	0.089
O (19)	0.021	0.020
O (20)	0.020	0.021
O (21)	0.076	0.073
H (22)	0.013	0.008
H (23)	0.018	0.012
H (24)	0.021	0.016
H (25)	0.036	0.022
H (26)	0.040	0.026
H (27)	0.041	0.027
H (28)	0.036	0.022
H (29)	0.026	0.029
H (30)	0.005	0.007
H (31)	0.009	0.009
H (32)	0.024	0.024

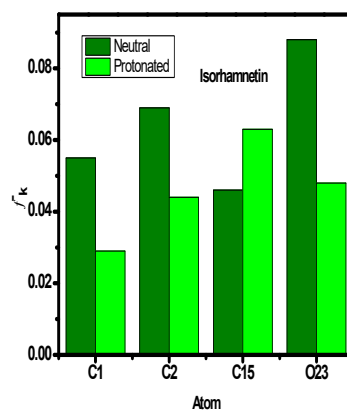
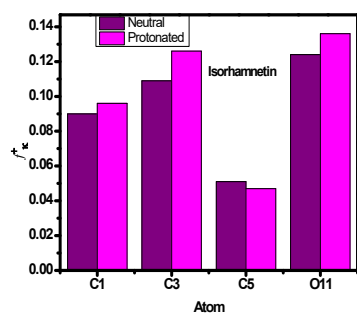


Fig. S10. Graphical representation of the Fukui indices of Isorhamnetin for the more reactive atoms in the un-protonated and protonated form.

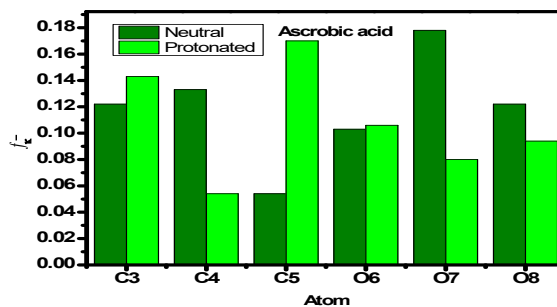
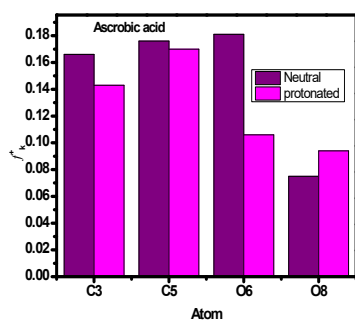


Fig. S11. Graphical representation of the Fukui indices of Ascorbic acid for the more reactive atoms in the un-protonated and protonated form.

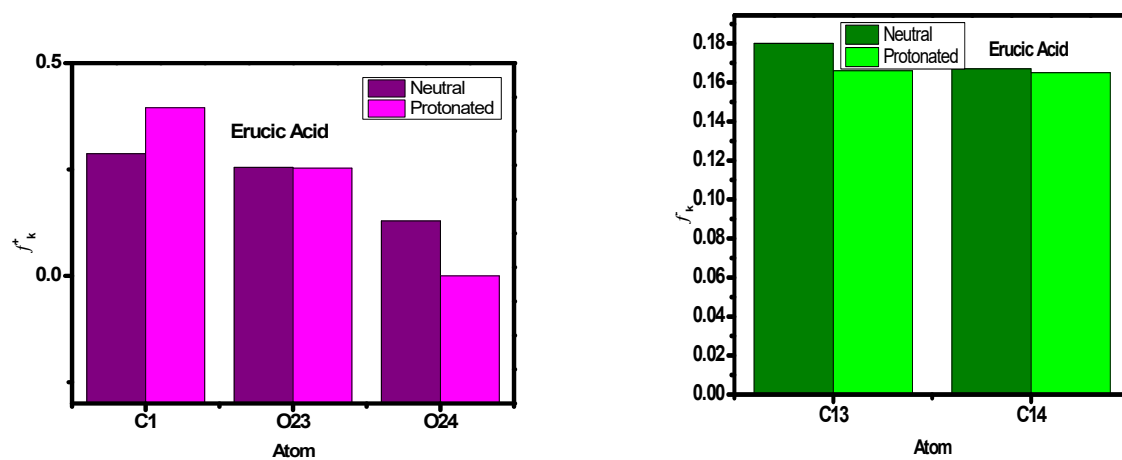


Fig. S13. Graphical representation of the Fukui indices of Erucic acid for the more reactive atoms in the unprotonated and protonated form.

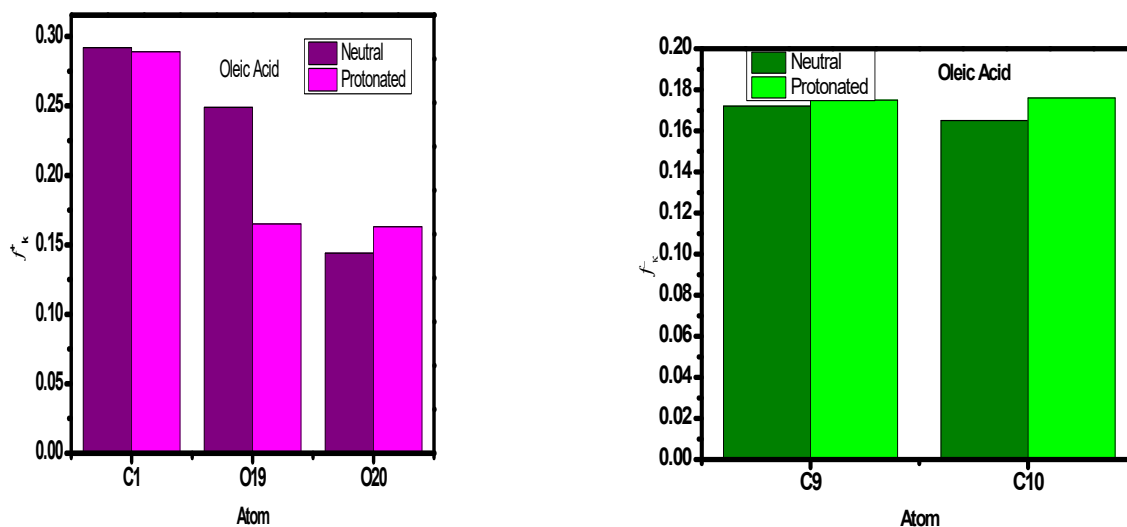
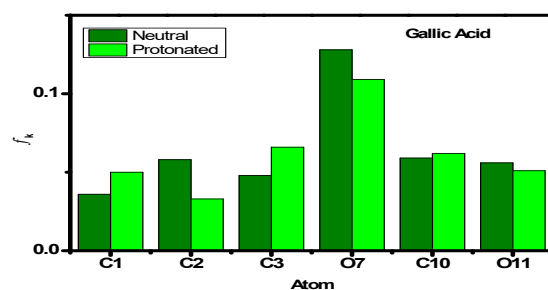


Fig. S14. Graphical representation of the Fukui indices of Oleic acid for the more reactive atoms in the unprotonated and protonated form.



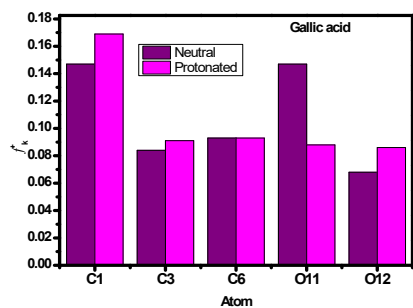


Fig. S15. Graphical representation of the Fukui indices of Gallic acid for the more reactive atoms in the unprotonated and protonated form.

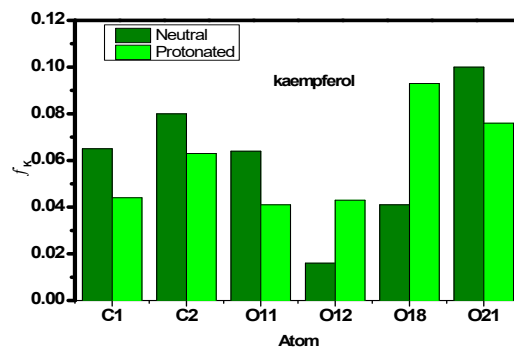
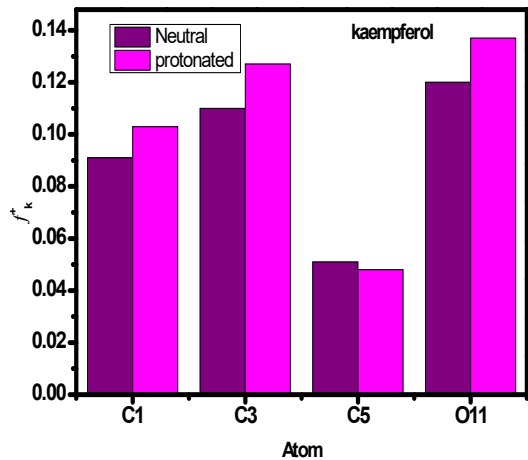


Fig. S16. Graphical representation of the Fukui indices of kaempferol acid for the more reactive atoms in the unprotonated and protonated form.