Use of Swiss Chard stems and Green Pea Peel extracts as anticorrosive agents for Aluminum in 1M HCl

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Appendix A: Supplementary figures

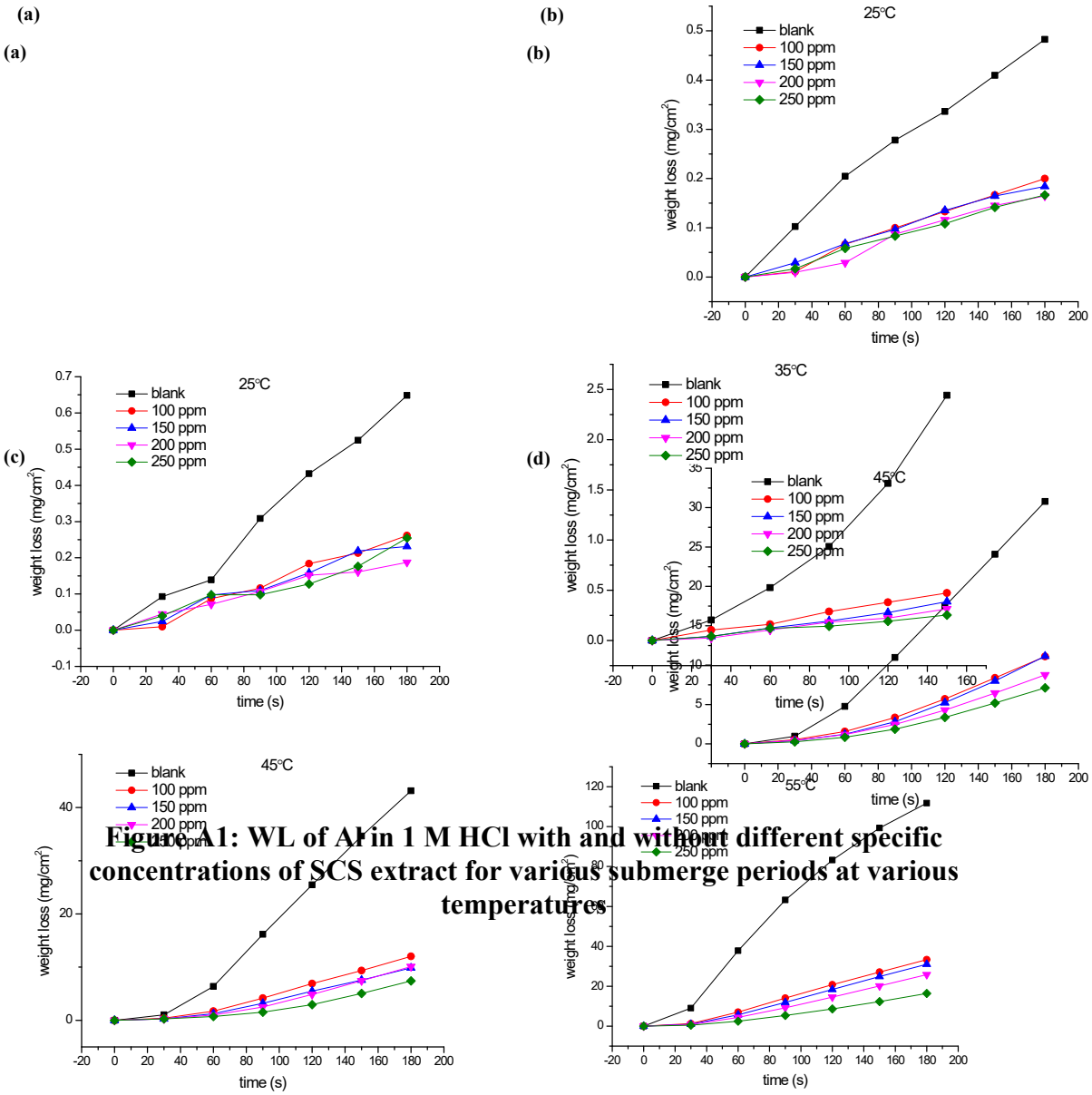


Figure A1: WL of Al in 1 M HCl with and without different specific concentrations of SCS extract for various submerge periods at various temperatures

Figure A2: WL of Al in 1 M HCl with and without different specific concentrations of GPP extract for various submerge periods at various temperatures

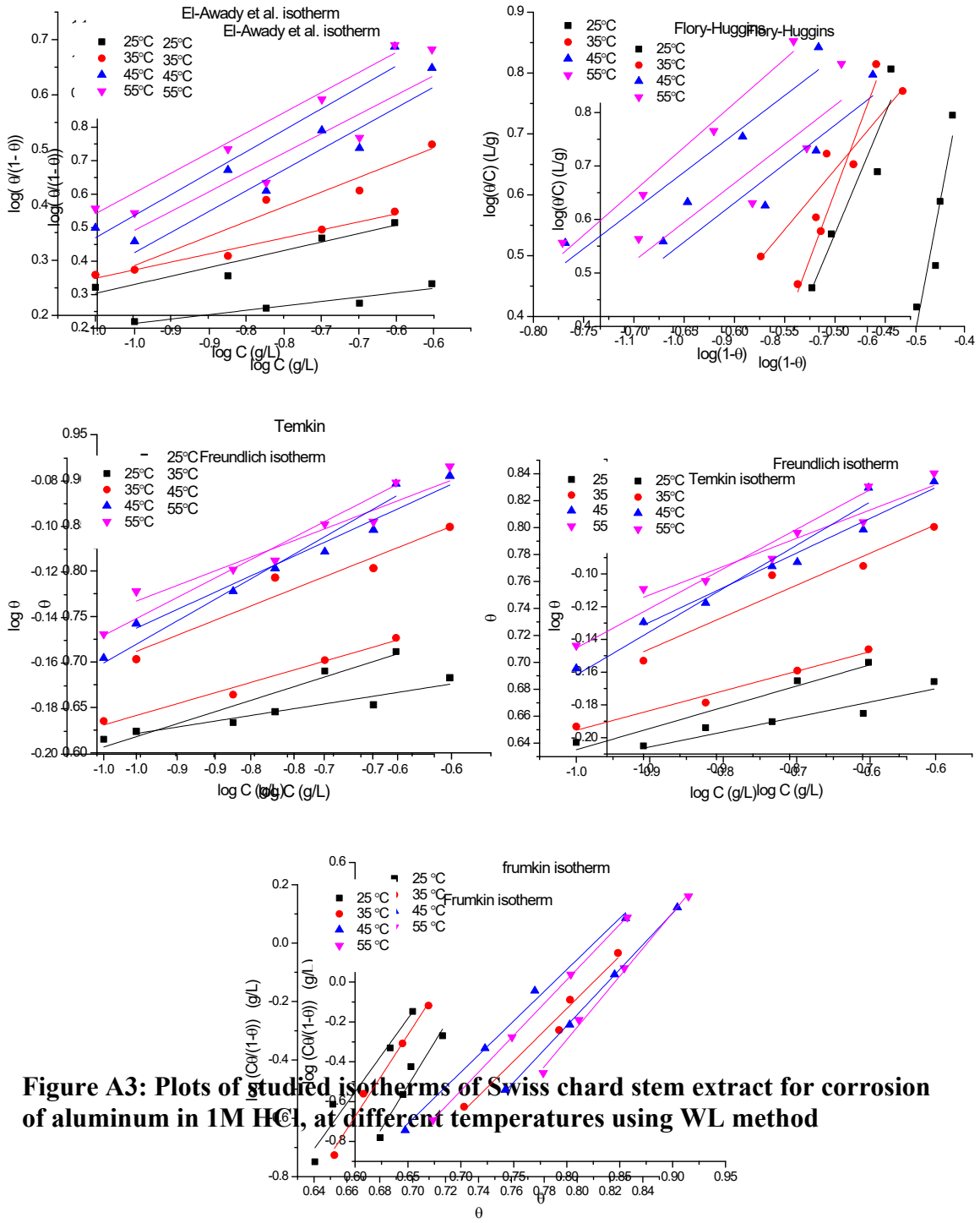
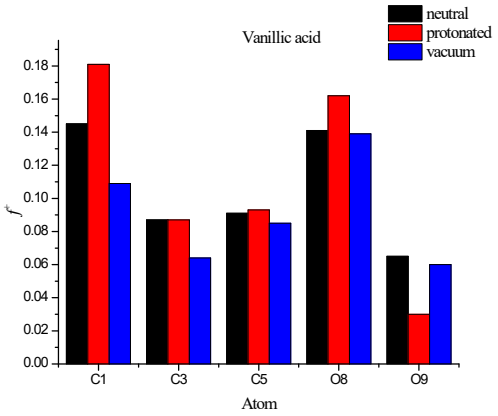
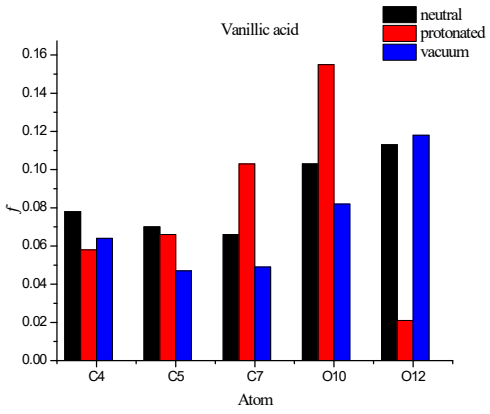
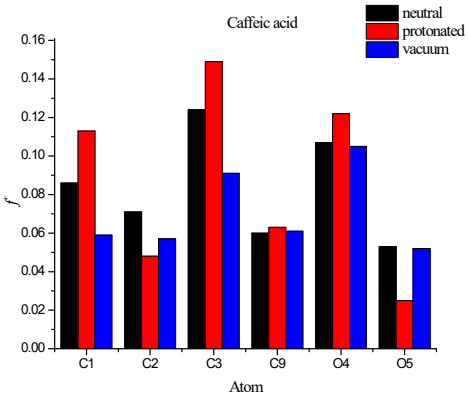


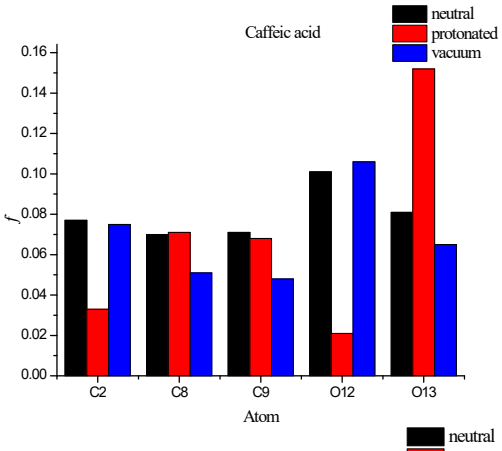
Figure A3: Plots of studied isotherms of Swiss chard stem extract for corrosion of aluminum in 1M HCl, at different temperatures using WL method

Figure A4: Plots of studied isotherms of green pea peels extract for corrosion of aluminum in 1M HCl, at different temperatures applying WL method

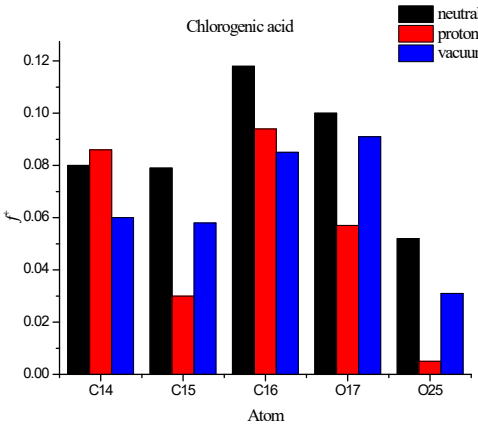

Vanillic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
C1
C3
C5
O8
O9
Atom


Vanillic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
C4
C5
C7
O10
O12
Atom


Caffeic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
C1
C2
C3
C9
O4
O5
Atom


Caffeic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
C2
C8
C9
O12
O13
Atom

(a)


Chlorogenic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
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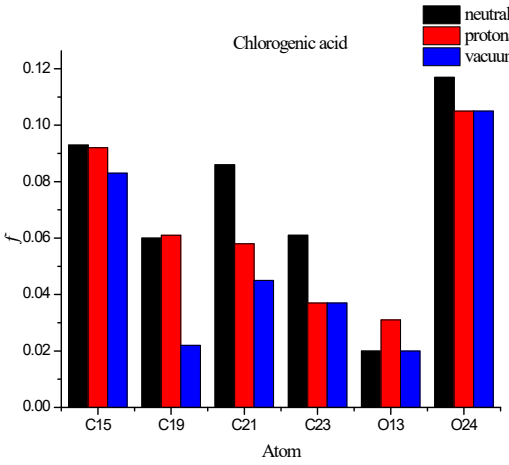
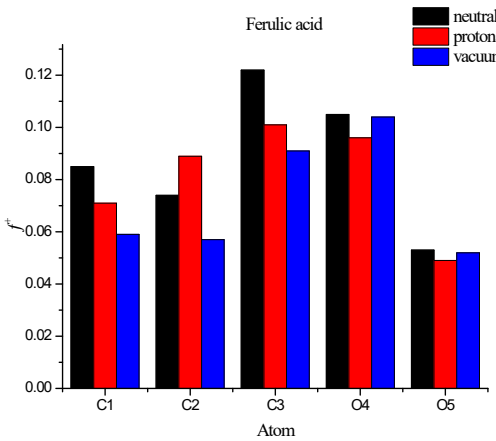
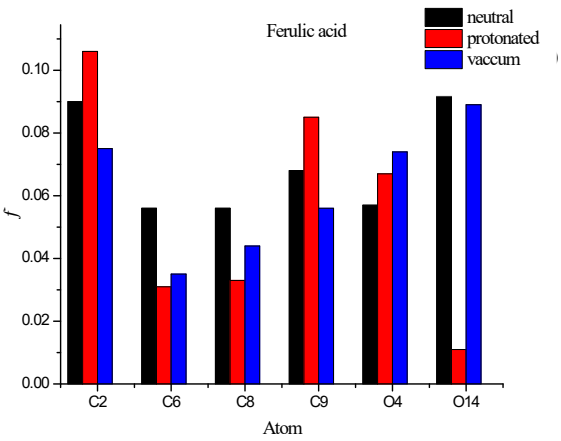
0.06
0.08
0.10
0.12
C14
C15
C16
O17
O25
Atom

(a`)


Chlorogenic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C15
C19
C21
C23
O13
O24
Atom

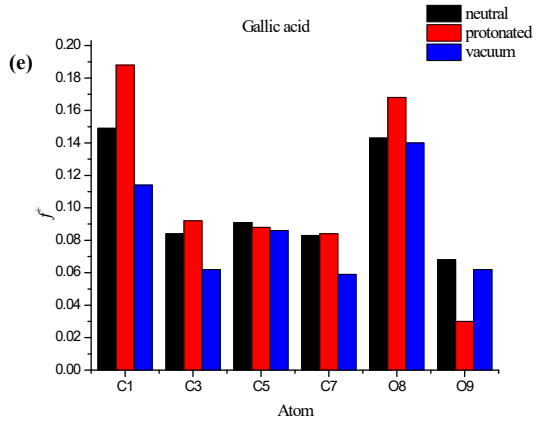
(b)

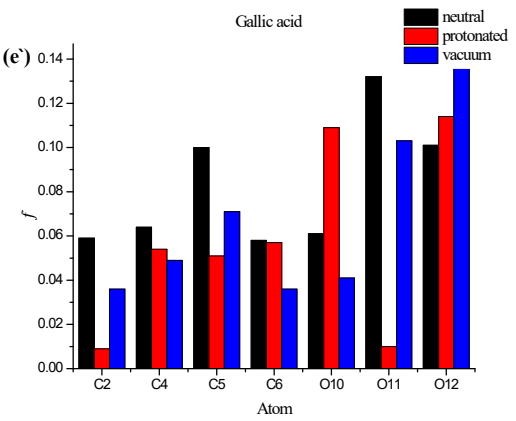

Ferulic acid
neutral
protonated
vacuum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C1
C2
C3
O4
O5
Atom

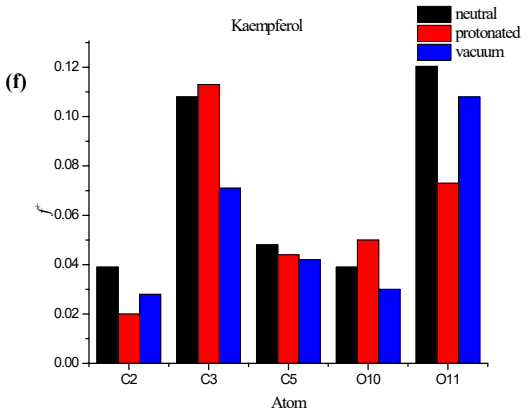

Ferulic acid
neutral
protonated
vaccum
f⁻
0.00
0.02
0.04
0.06
0.08
0.10
C2
C6
C8
C9
O4
O14
Atom

(c)

(c`)


(e)
Gallic acid
neutral
protonated
vacuum
f-
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C1
C3
C5
C7
O8
O9
Atom


(e`)
Gallic acid
neutral
protonated
vacuum
f-
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C2
C4
C5
C6
O10
O11
O12
Atom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Kaempferol
neutral
protonated
vacuum
f-
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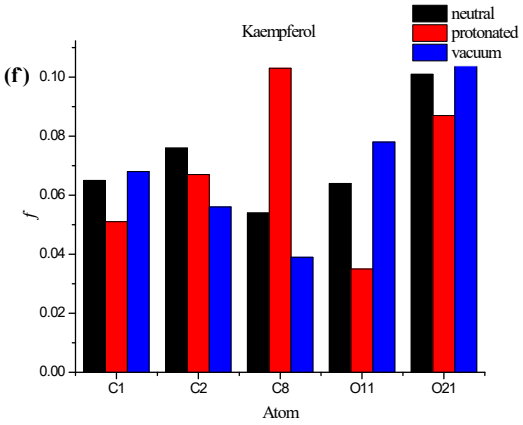
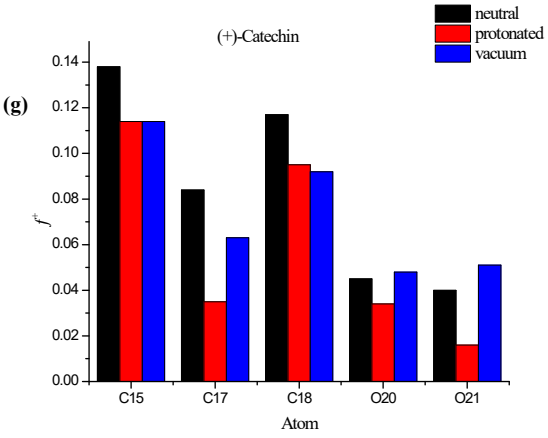
0.10
0.08
0.06
0.04
0.02
0.00
C2
C3
C5
O10
O11
Atom


(f`)
Kaempferol
neutral
protonated
vacuum
f-
0.10
0.08
0.06
0.04
0.02
0.00
C1
C2
C8
O11
O21
Atom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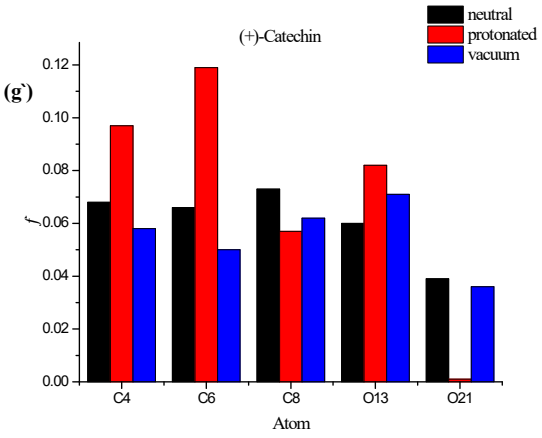
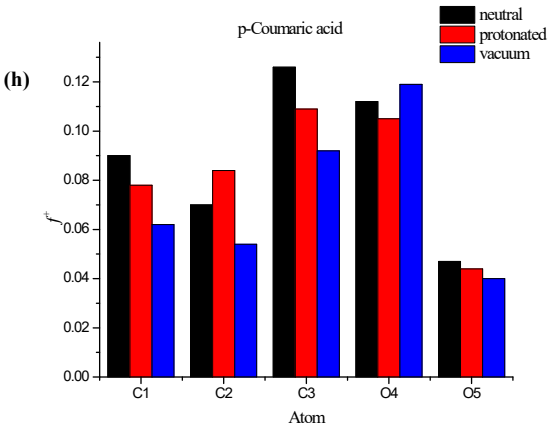
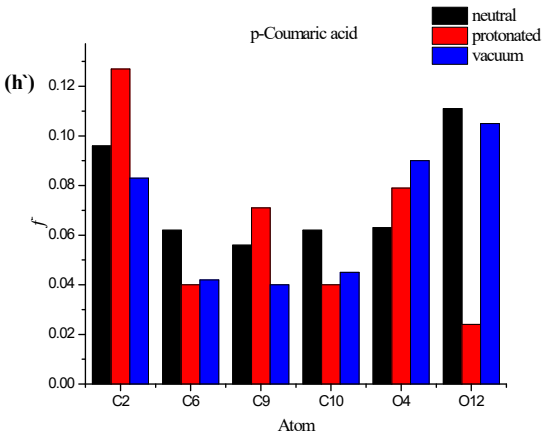
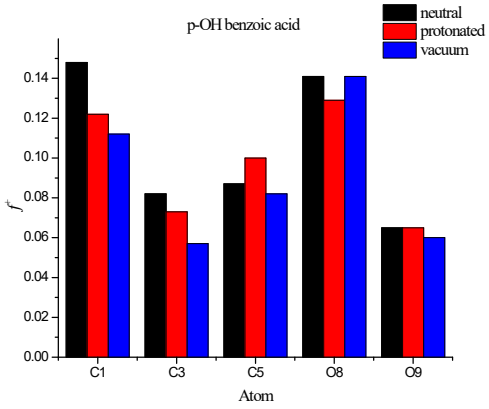
(+)-Catechin
neutral
protonated
vacuum
f+
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C15
C17
C18
O20
O21
Atom


(g`)
(+)-Catechin
neutral
protonated
vacuum
f-
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C4
C6
C8
O13
O21
Atom


(h)
p-Coumaric acid
neutral
protonated
vacuum
f+
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C1
C2
C3
O4
O5
Atom


(h`)
p-Coumaric acid
neutral
protonated
vacuum
f-
0.12
0.10
0.08
0.06
0.04
0.02
0.00
C2
C6
C9
C10
O4
O12
Atom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protonated
vacuum
f^-
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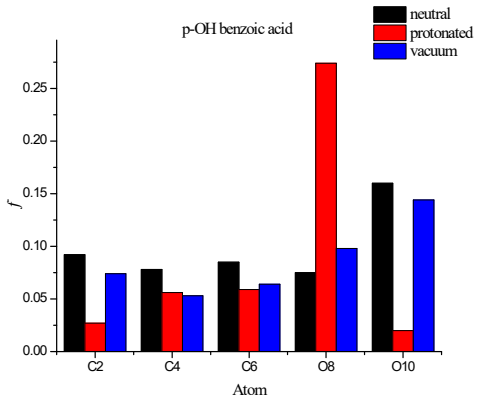
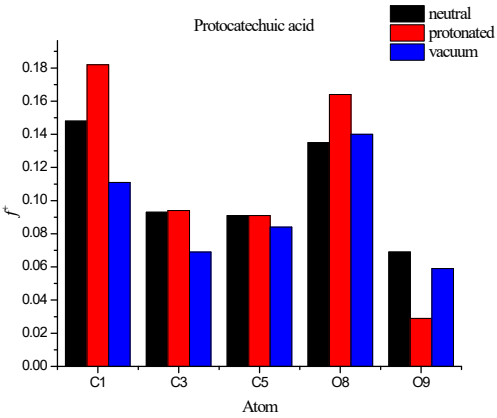
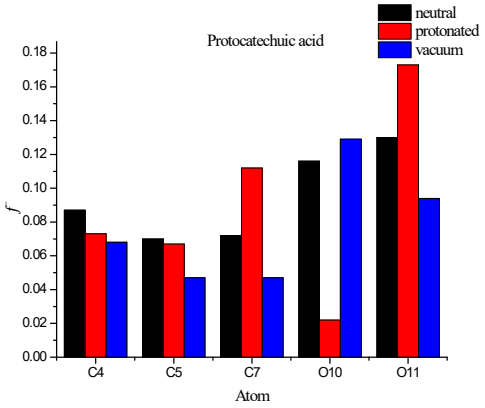
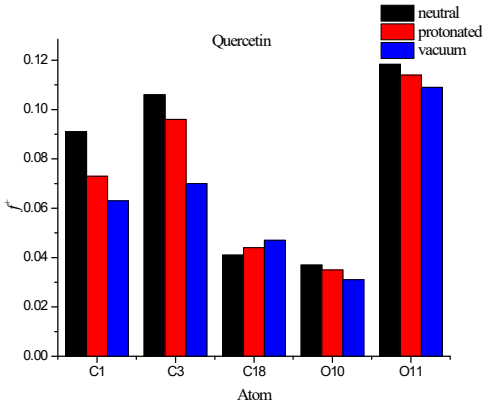
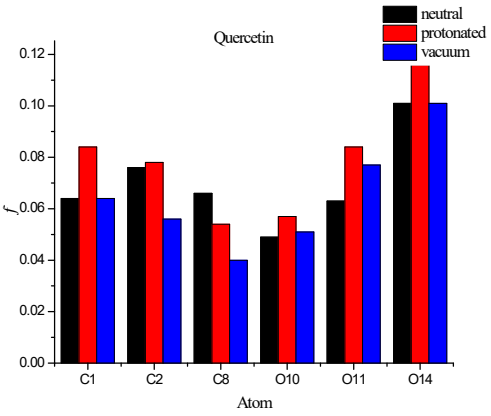
0.02
0.04
0.06
0.08
0.10
0.12
0.14
C1
C3
C5
O8
O9
Atom


p-OH benzoic acid
neutral
protonated
vacuum
f^-
0.00
0.05
0.10
0.15
0.20
0.25
C2
C4
C6
O8
O10
Atom

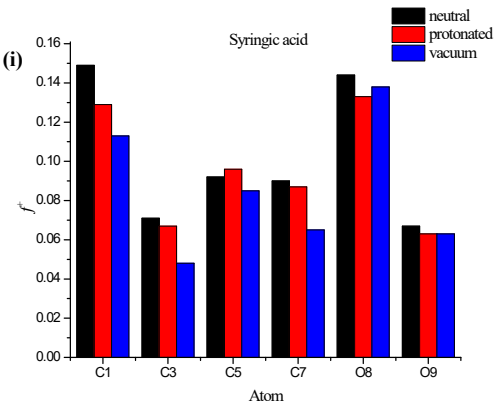

Protocatechuic acid
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
C1
C3
C5
O8
O9
Atom


Protocatechuic acid
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
C4
C5
C7
O10
O11
Atom


Quercetin
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C1
C3
C18
O10
O11
Atom


Quercetin
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C1
C2
C8
O10
O11
O14
Atom

(i)


Syringic acid
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
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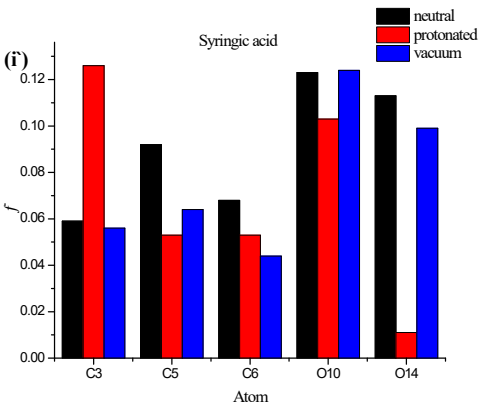
0.12
0.14
0.16
C1
C3
C5
C7
O8
O9
Atom

(i`)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protonated
vacuum
f^-
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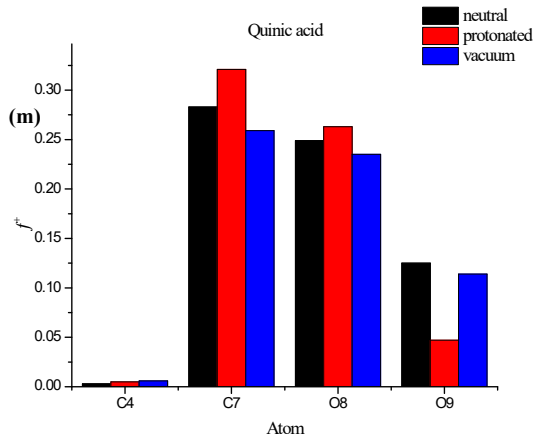
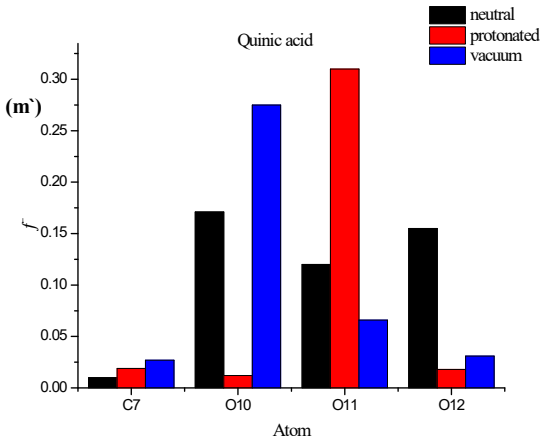
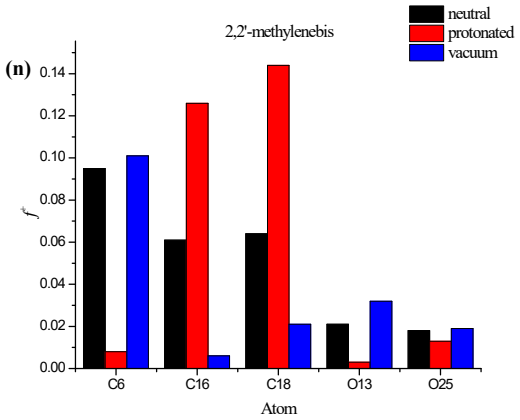
0.12
C3
C5
C6
O10
O14
Atom

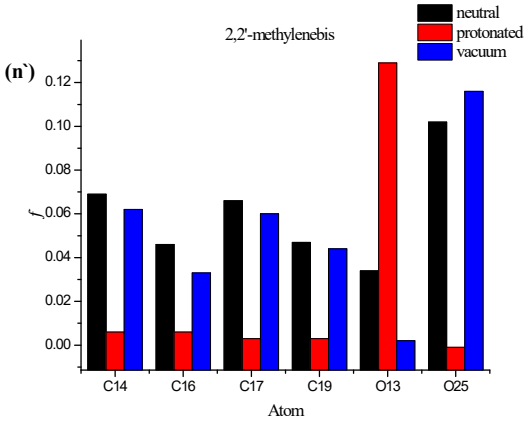
(j)

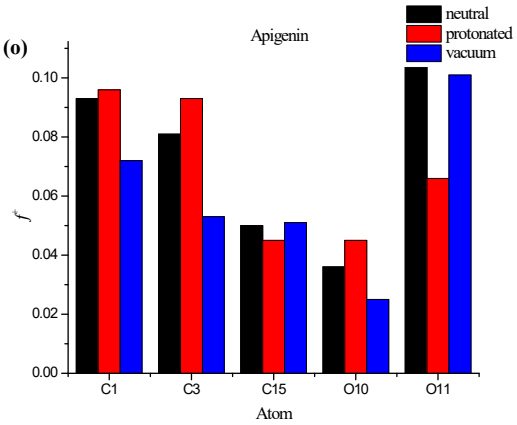
8(j`)

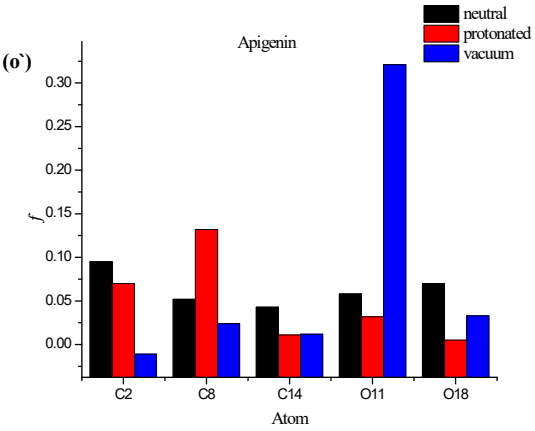

(m)
Quinic acid
neutral
protonated
vacuum
f^0
0.00
0.05
0.10
0.15
0.20
0.25
0.30
C4
C7
O8
O9
Atom

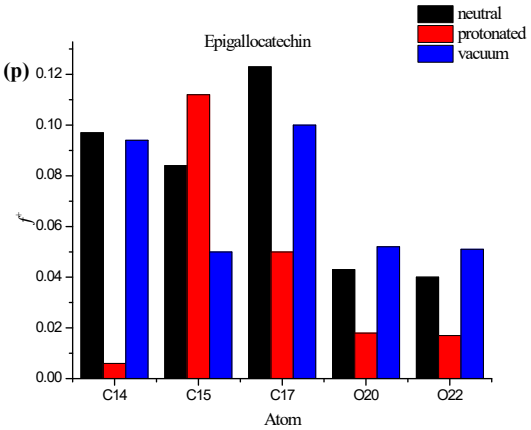

(m`)
Quinic acid
neutral
protonated
vacuum
f^-
0.00
0.05
0.10
0.15
0.20
0.25
0.30
C7
O10
O11
O12
Atom

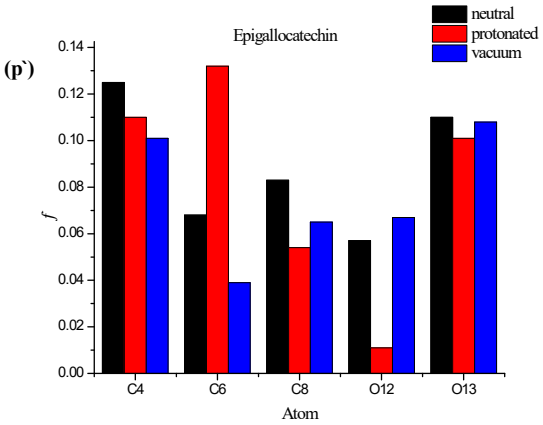

(n)
2,2'-methylenebis
neutral
protonated
vacuum
f^0
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
C6
C16
C18
O13
O25
Atom


(n`)
2,2'-methylenebis
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C14
C16
C17
C19
O13
O25
Atom


(o)
Apigenin
neutral
protonated
vacuum
f^0
0.00
0.02
0.04
0.06
0.08
0.10
C1
C3
C15
O10
O11
Atom


(o`)
Apigenin
neutral
protonated
vacuum
f^-
0.00
0.05
0.10
0.15
0.20
0.25
0.30
C2
C8
C14
O11
O18
Atom


(p)
Epigallocatechin
neutral
protonated
vacuum
f^0
0.00
0.02
0.04
0.06
0.08
0.10
0.12
C14
C15
C17
O20
O22
Atom


(p`)
Epigallocatechin
neutral
protonated
vacuum
f^-
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
C4
C6
C8
O12
O13
Atom

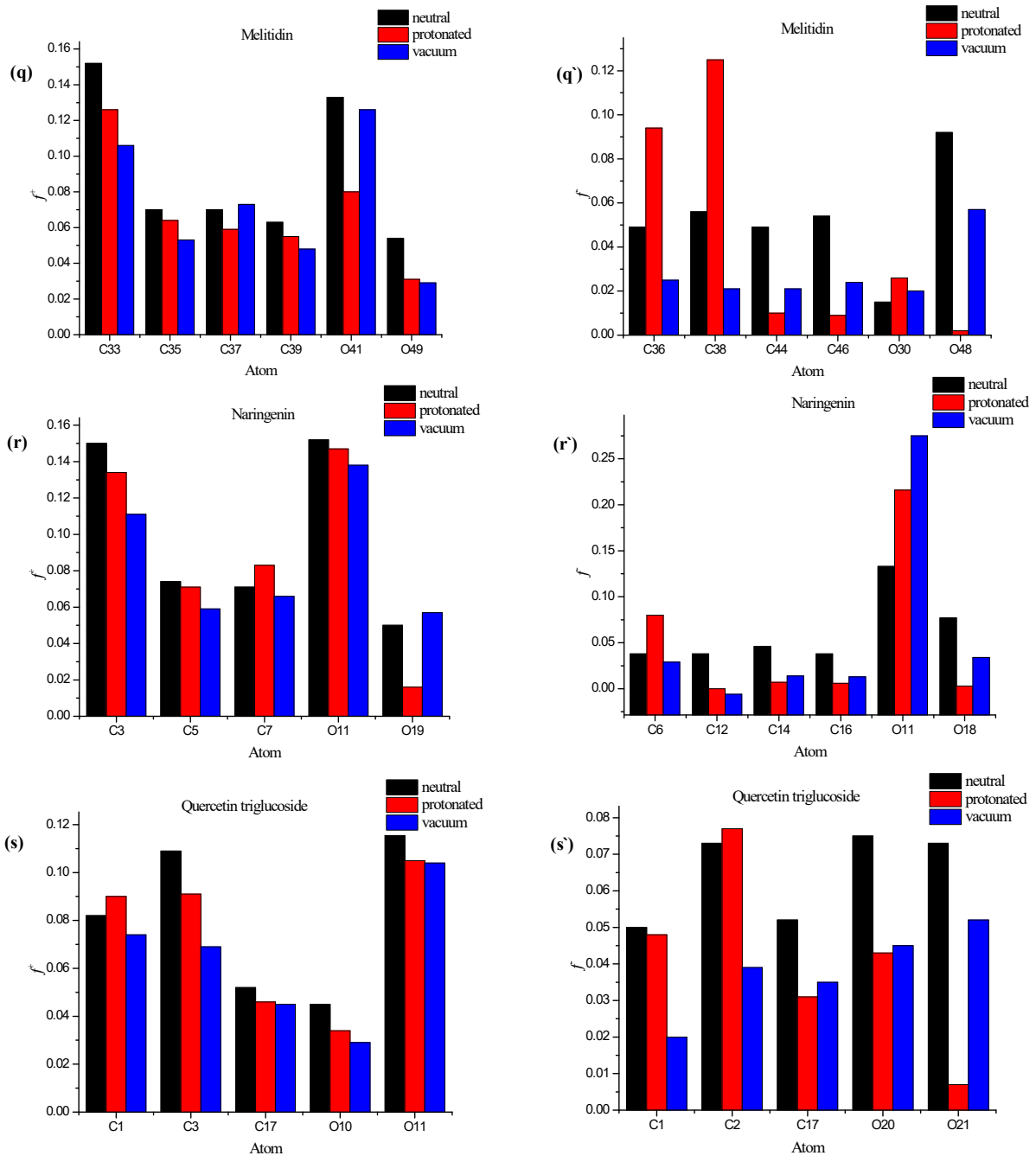


Figure A5: A graphic depiction of SCS and GPP compounds' Fukui indices for their more reactive atoms in both their protonated and non-protonated systems

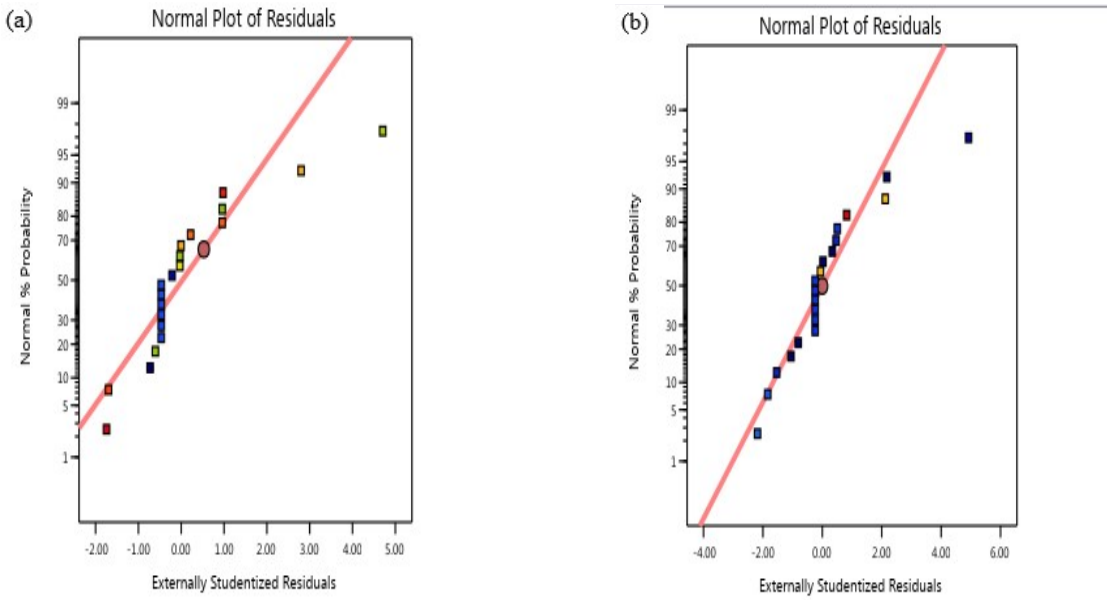


Figure A6: The normal probability plots for the externally studentized residuals of the corrosion inhibition efficiency (CIE) and corrosion rate (CR) models of GPP extract

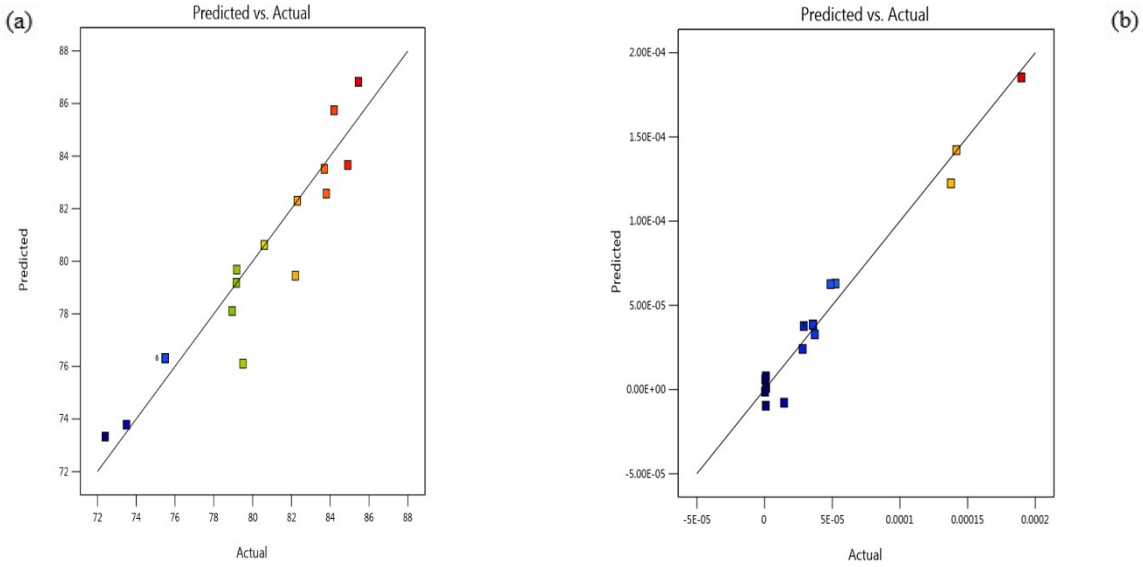


Figure A7: Plot of predicted versus actual values for the (a) inhibition efficiency model and (b) corrosion rate model of GPP extract

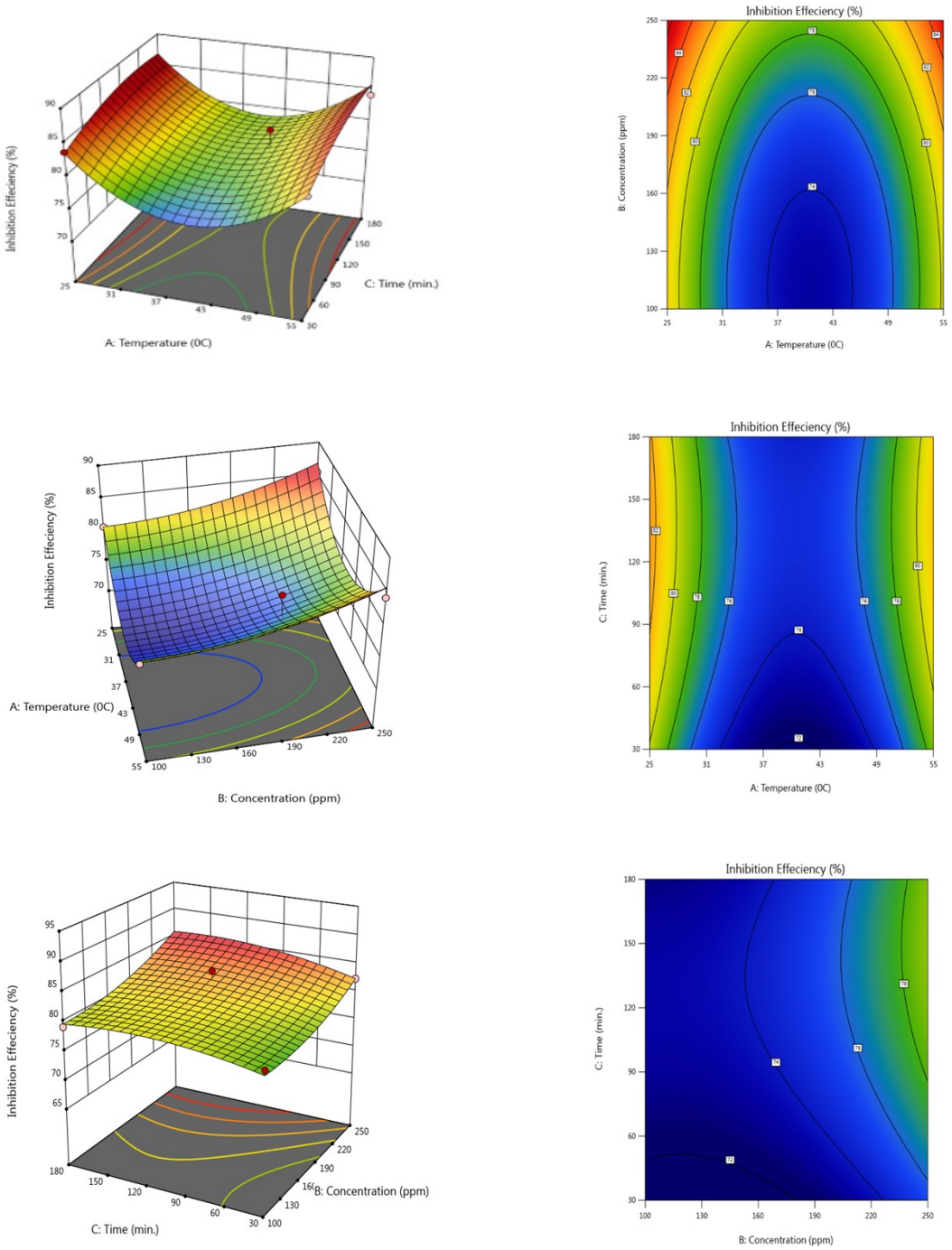


Figure A8: Interaction of variables' effects on the effectiveness of inhibition of GPP extract

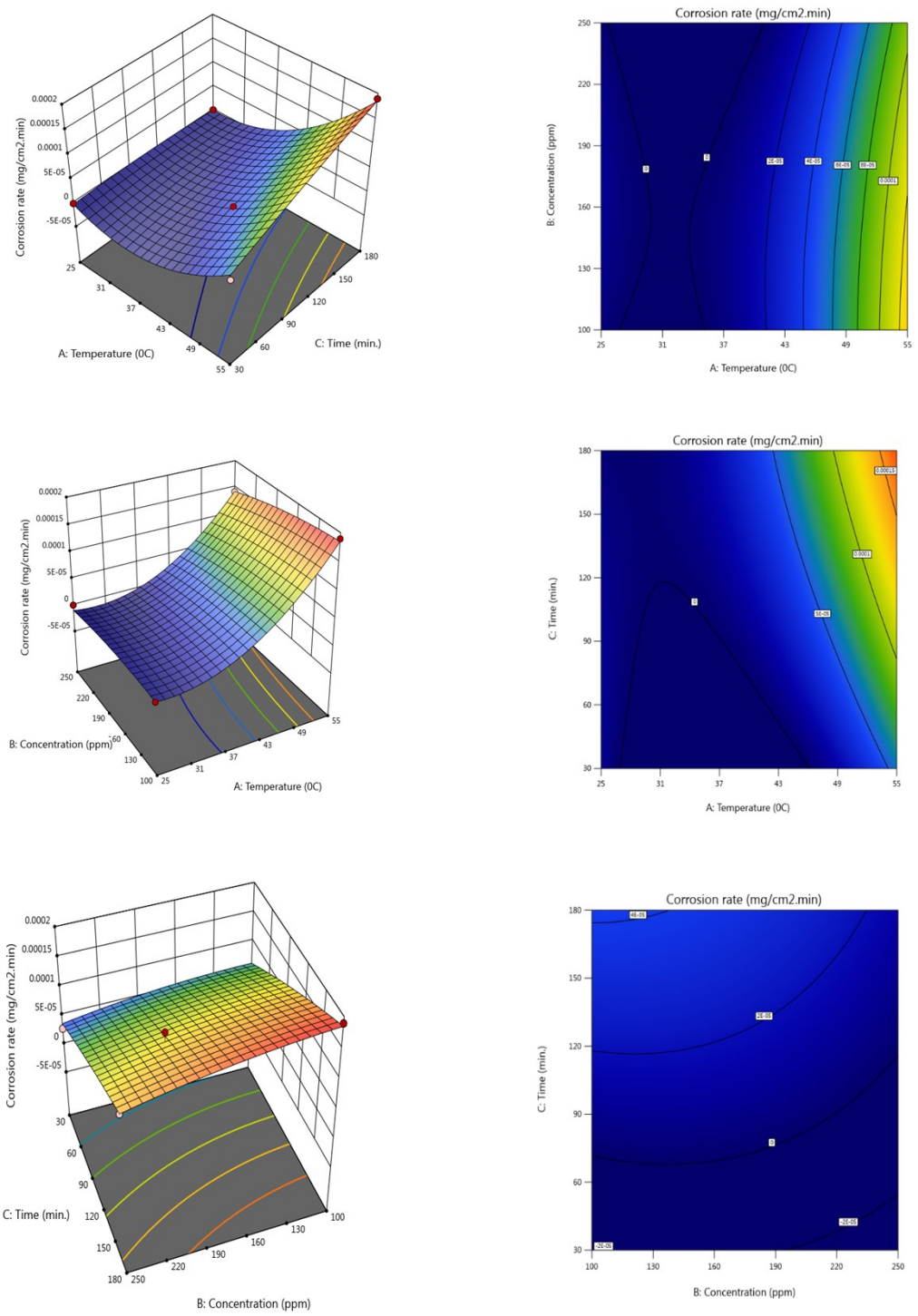


Figure A9: Interaction of variables' effects on the rate of corrosion after using GPP extract

Appendix B: Supplementary tables

Table B1: The important components of SCS extract

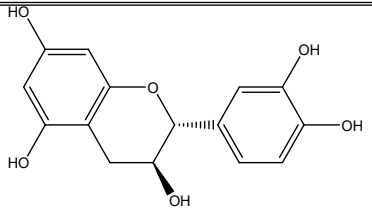
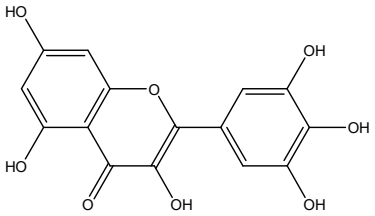
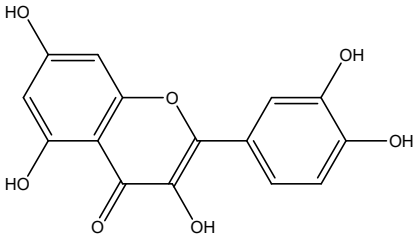
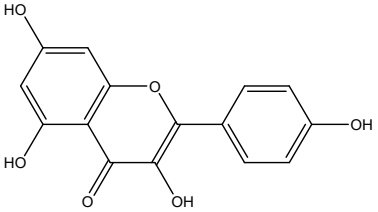
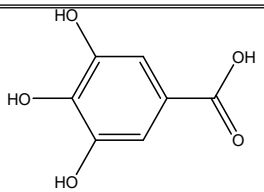
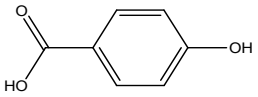
Constituents	Name	Chemical structure	Molecular weight (g/mol)
Flavonoids	(+)Catechin	 (2R,3S)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol	290.271
	Myricetin	 3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)chromen-4-one	318.23
	Quercetin	 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one	302.23
	Kaempferol	 3,5,7-trihydroxy-2-(4-hydroxyphenyl)chromen-4-one	286.24
Phenolicacids	Gallic acid	 3,4,5-trihydroxybenzoic acid	170.12
	p-OH-benzoic acid	 4-hydroxybenzoic acid	138.12

Table B1 (continued)

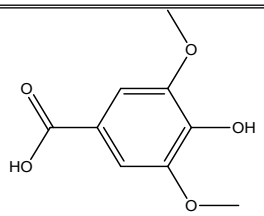
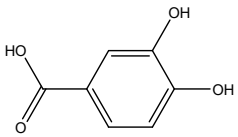
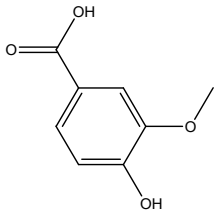
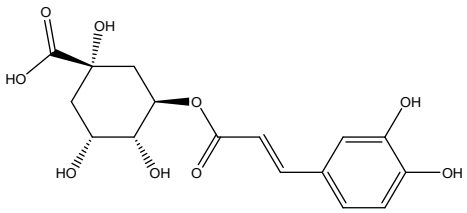
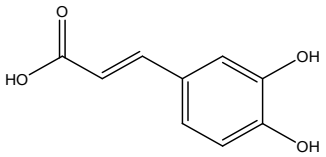
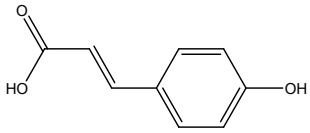
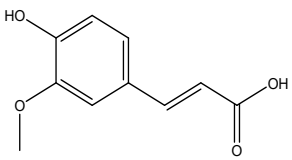
Constituents	Name	Chemical structure	Molecular weight (g/mol)
Phenolicacids	Syringic acid	 4-hydroxy-3,5-dimethoxybenzoic acid	198.17
	Protocatechuic acid	 3,4-dihydroxybenzoic acid	154.12
	Vanillic acid	 4-hydroxy-3-methoxybenzoic acid	168.15
	Chlorogenic acid	 (1S,3R,4R,5R)-3-[(E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy-1,4,5-trihydroxycyclohexane-1-carboxylic acid	354.31
	Caffeic acid	 (E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid	180.16
	p-Coumaric acid	 (E)-3-(4-hydroxyphenyl)prop-2-enoic acid	164.16
	Ferulic acid	 (E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid	194.18

Table B2: The important components of GPP extract

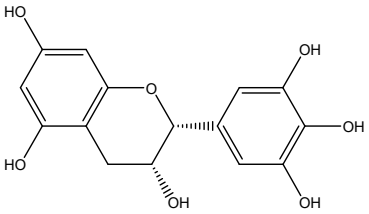
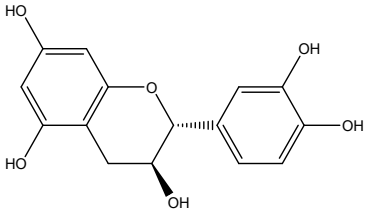
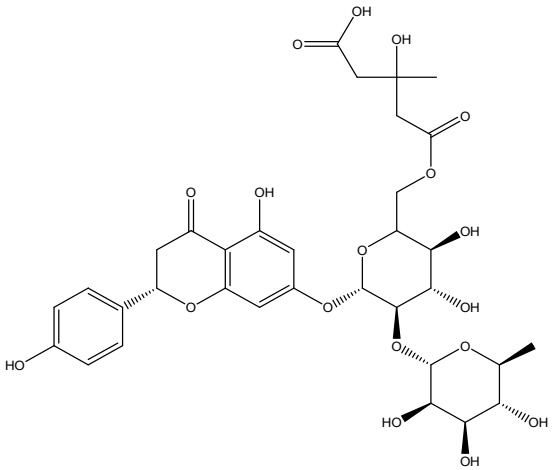
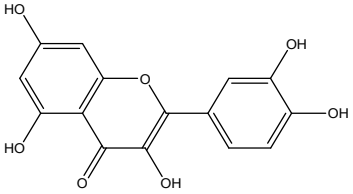
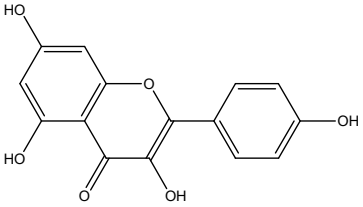
Constituents	Name	Chemical structure	Molecular weight (g/mol)
Flavonoids	(Epi)gallocatechin	 (2R,3R)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol	306.27
	Catechin	 (2R,3S)-2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2H-chromene-3,5,7-triol	290.271
	Melitidin	 5-[[(2R,3S,4S,5R,6S)-3,4-dihydroxy-6-[[(2S)-5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-2,3-dihydrochromen-7-yl]oxy]-5-[(2S,3R,4R,5R,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxyoxan-2-yl]methoxy]-3-hydroxy-3-methyl-5-oxopentanoic acid	724.7
	Quercetin	 2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxychromen-4-one	302.23
	Kaempferol	 3,5,7-trihydroxy-2-(4-hydroxyphenyl)chromen-4-one	286.24

Table B2 (continued)

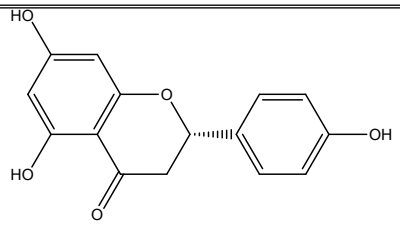
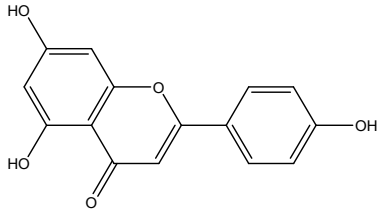
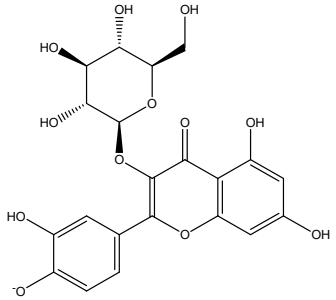
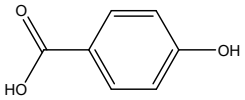
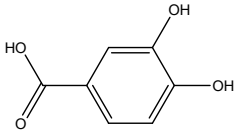
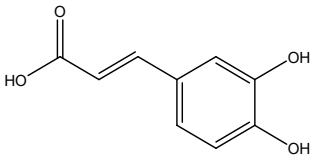
Constituents	Name	Chemical structure	Molecular weight (g/mol)
Flavonoids	Naringenin	 (2S)-5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydrochromen-4-one	272.25
	Apigenin	 5,7-dihydroxy-2-(4-hydroxyphenyl)chromen-4-one	270.24
	Quercetin 3-glucoside	 4-[5,7-dihydroxy-4-oxo-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxychromen-2-yl]-2-hydroxyphenolate	463.4
phenolic compounds	p-Hydroxybenzoic acid	 4-hydroxybenzoic acid	138.12
	Protocatechuic acid	 3,4-dihydroxybenzoic acid	154.12
	Caffeic acid	 (E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid	180.16

Table B2 (continued)

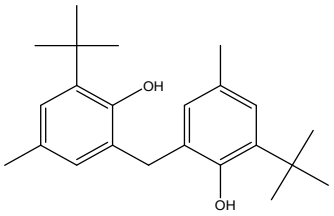
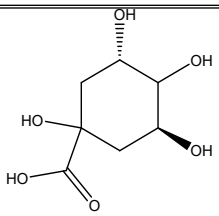
Constituents	Name	Chemical structure	Molecular weight (g/mol)
phenolic compounds	2,2'-methylenebis (4-methyl-6-tert-butylphenol)	 2,2'-methylenebis(4-methyl-6-tert-butylphenol)	340.5
Non-phenolics	Quinic acid	 (3S,5S)-1,3,4,5-tetrahydroxycyclohexane-1-carboxylic acid	192.17

Table B3: Correlation coefficient (R^2) for different adsorption isotherms for adsorption of SCS extract on the Al surface at different temperatures after 90 minutes' immersion time

	25 ℃	35 ℃	45 ℃	55 ℃
El-Awady et al.	0.8685	0.92358	0.9024	0.80029
Flory-Huggins	0.83162	0.88291	0.85506	0.72044
Freundlich	0.88777	0.90493	0.98261	0.91414
Frumkin	0.92507	0.96857	0.99946	0.99425
Henry	0.93101	0.84527	0.97353	0.99331
Langmuir	0.99457	0.99585	0.99055	0.99688
Temkin	0.8778	0.91336	0.97231	0.89691

Table B4: Correlation coefficient (R^2) for different adsorption isotherms for adsorption of GPP extract on the Al surface at different temperatures after 90 minutes' immersion time

	25 ℃	35 ℃	45 ℃	55 ℃
El-Awady et al.	0.8841	0.96468	0.90996	0.98112
Flory-Huggins	0.85329	0.95331	0.86001	0.9699
Freundlich	0.89103	0.97297	0.96176	0.99822
Frumkin	0.93534	0.98233	0.99115	0.99986
Henry	0.99144	0.93452	0.98961	0.98357
Langmuir	0.99342	0.99869	0.99776	0.99915
Temkin	0.8875	0.96922	0.94873	0.99533

Table B5: The HOMO and LUMO orbital distribution and molecular structure optimization for important components in SCS and GPP extracts were determined via the DMol^3/GGA/BOP approach (protonated)

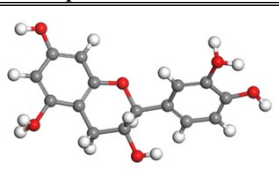
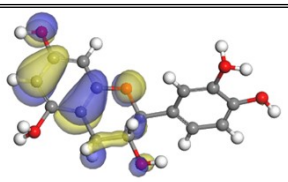
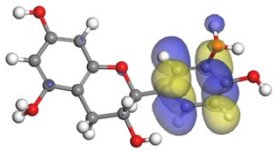
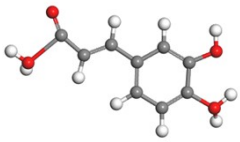
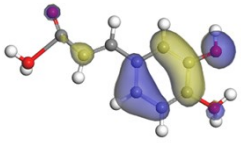
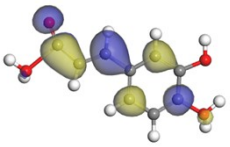
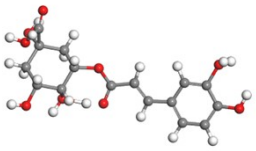
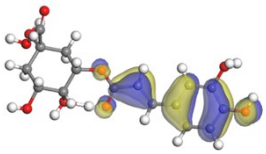
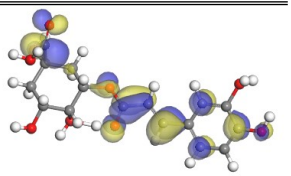
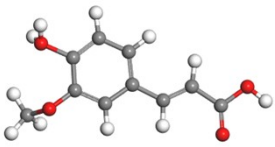
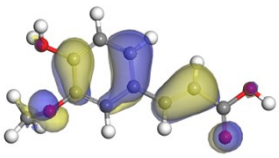
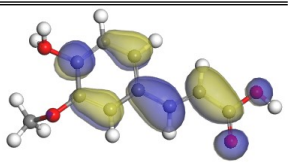
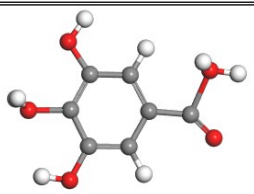
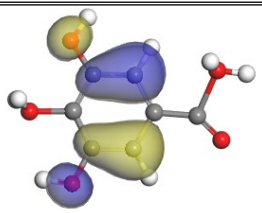
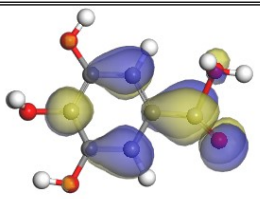
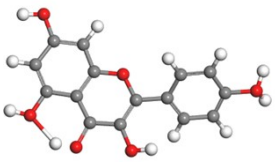
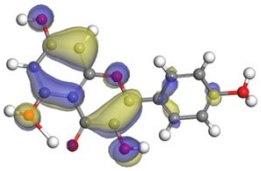
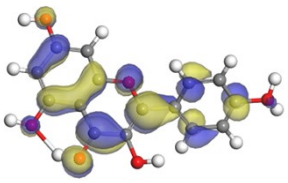
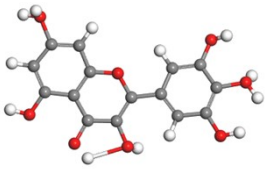
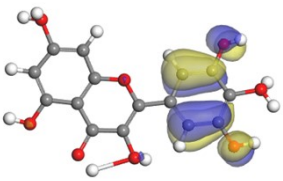
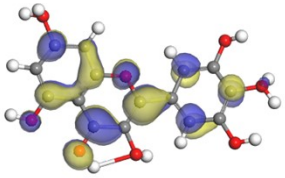
Compound	Optimized structure	HOMO	LUMO
(+)- Catechin			
Caffeic acid			
Chlorogenic acid			
Ferulic acid			
Gallic acid			
Kaempferol			
Myricetin			

Table B5 (continued)

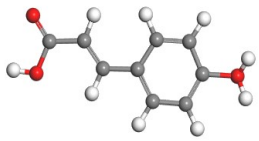
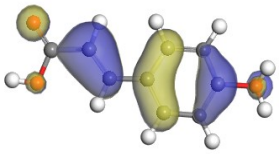
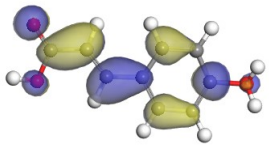
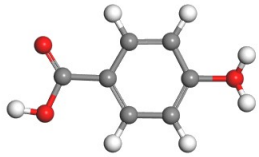
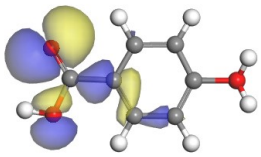
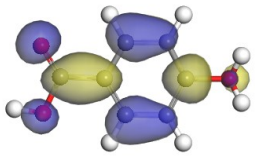
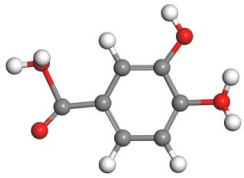
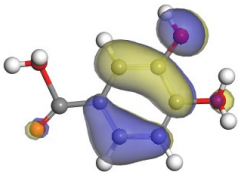
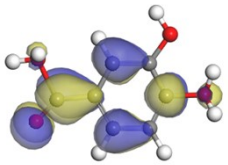
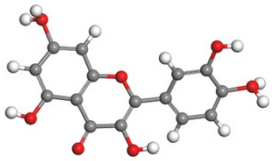
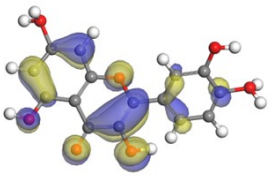
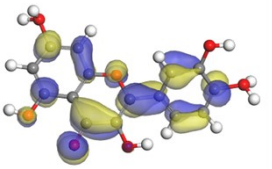
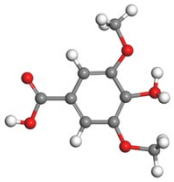
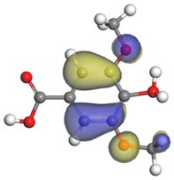
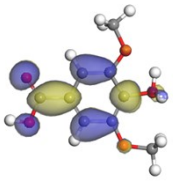
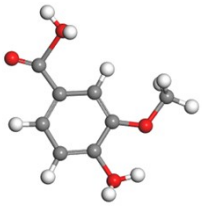
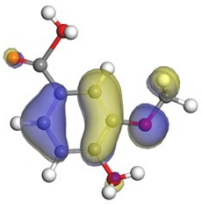
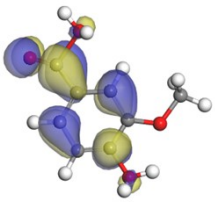
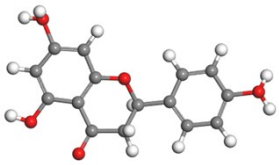
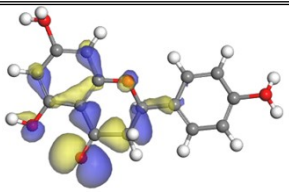
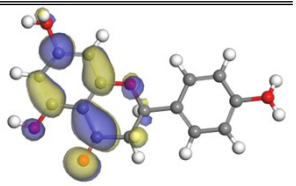
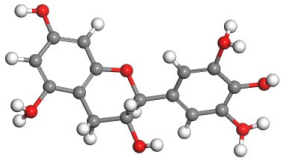
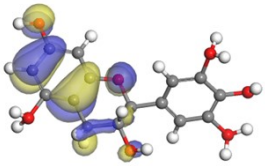
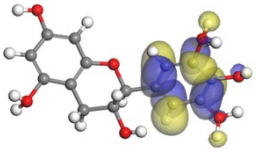
Compound	Optimized structure	HOMO	LUMO
p- coumaric acid			
p-OH benzoic acid			
Protocatechuic acid			
Quercetin			
Syringic acid			
Vanillic acid			
Naringenin			
Epigallocatechin			

Table B5 (continued)

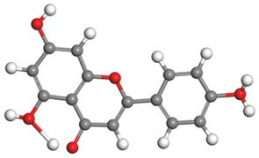
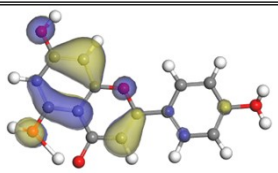
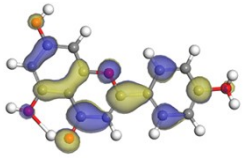
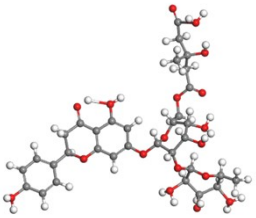
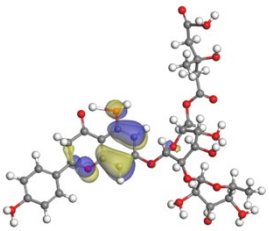
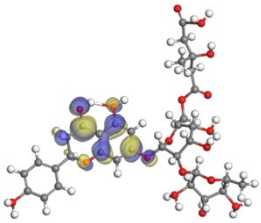
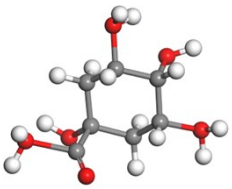
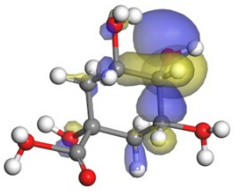
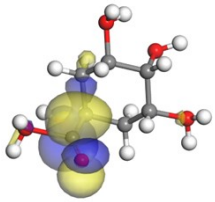
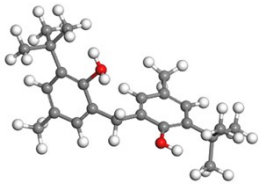
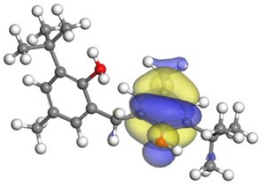
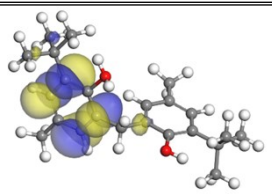
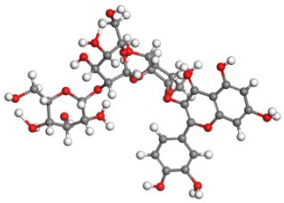
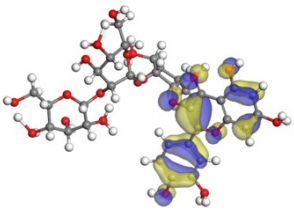
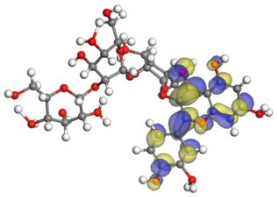
Compound	Optimized structure	HOMO	LUMO
Apigenin			
Melitidin			
Quinic acid			
2,2'-methylenebis			
Quercetin triglucoside			

Table B6: The quantum data for Swiss chard stems extract in the neutral, protonated, and vacuum form

	(+)- Catechin			Caffeic acid			Chlorogenic acid			Ferulic acid			Gallic acid		
	Neutral	Protonated	Vacuum	Neutral	Protonated	Vacuum	Neutral	Protonated	Vacuum	Neutral	Protonated	Vacuum	Neutral	Protonated	Vacuum
E_{HOMO} (eV)	-4.905	-5.566	-4.395	-4.923	-6.39	-4.565	-5.08	-6.136	-4.67	-5.065	-6.042	-4.64	-5.161	-6.322	-4.726
E_{LUMO} (eV)	-0.766	-1.623	-0.285	-2.331	-4.119	-1.807	-2.332	-3.645	-1.912	-2.342	-2.867	-1.784	-1.86	-3.82	-1.285
Dipole moment (Debye)	2.205	6.260	1.557	3.481	5.731	2.495	5.548	17.900	2.716	6.384	17.633	4.648	6.440	6.867	4.470
Molecular area ($Å^2$)	286.978	294.426		203.469	211.438		348.105	352.427		222.080	224.652		178.283	187.526	
ΔE (eV)	4.139	3.943	4.11	2.592	2.271	2.758	2.748	2.491	2.758	2.723	3.175	2.856	3.301	2.502	3.441
η (eV)	2.070	1.972	2.055	1.296	1.136	1.379	1.374	1.246	1.379	1.362	1.588	1.428	1.651	1.251	1.721
σ $(eV)^{-1}$	0.483	0.507	0.487	0.772	0.881	0.725	0.728	0.803	0.725	0.734	0.630	0.700	0.606	0.799	0.581
Pi (eV)	-2.836	-3.595	-2.340	-3.627	-5.255	-3.186	-3.706	-4.891	-3.291	-3.704	-4.455	-3.212	-3.511	-5.071	-3.006
χ (eV)	2.836	3.595	2.340	3.627	5.255	3.186	3.706	4.891	3.291	3.704	4.455	3.212	3.511	5.071	3.006
ω	1.943	3.277	1.332	5.075	12.158	3.680	4.998	9.601	3.927	5.037	6.250	3.612	3.733	10.278	2.625
ω^+	0.783	1.726	0.419	3.424	9.672	2.260	3.317	7.312	2.454	3.355	4.221	2.185	2.184	7.899	1.337
ω^-	3.619	5.320	2.759	7.051	14.927	5.446	7.023	12.202	5.745	7.059	8.675	5.397	5.695	12.970	4.343
ε	0.515	0.305	0.751	0.197	0.082	0.272	0.200	0.104	0.255	0.199	0.160	0.277	0.268	0.097	0.381
ΔE back donation	-0.517	-0.493	-0.514	-0.324	-0.284	-0.345	-0.344	-0.311	-0.345	-0.340	-0.397	-0.357	-0.413	-0.313	-0.430
ΔN_{max} (e)	0.095	-0.092	0.217	-0.153	-0.891	0.016	-0.173	-0.667	-0.022	-0.174	-0.386	0.006	-0.085	-0.736	0.065

Table B6 (continued)

	Kaempferol			Myricetin			p- coumaric acid			p-OH benzoic acid		
	Neutral	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**
E_{HOMO} (eV)	-4.8	-5.737	-4.237	-4.899	-6.25	-4.309	-5.092	-5.991	-4.725	-5.47	-6.541	-5.022
E_{LUMO} (eV)	-2.105	-3.512	-1.462	-2.162	-4.031	-1.576	-2.319	-2.784	-1.801	-1.813	-2.483	-1.232
Dipole moment (Debye)	8.625	14.828	5.481	7.113	9.564	4.548	5.180	20.273	3.601	3.031	14.129	2.141
Molecular area ($Å^2$)	277.675	279.531		295.848	301.887		195.372	197.472		161.714	164.811	
ΔE (eV)	2.695	2.225	2.775	2.737	2.219	2.733	2.773	3.207	2.924	3.657	4.058	3.79
η (eV)	1.348	1.113	1.388	1.369	1.110	1.367	1.387	1.604	1.462	1.829	2.029	1.895
σ $(eV)^{-1}$	0.742	0.899	0.721	0.731	0.901	0.732	0.721	0.624	0.684	0.547	0.493	0.528
Pi (eV)	-3.453	-4.625	-2.850	-3.531	-5.141	-2.943	-3.706	-4.388	-3.263	-3.642	-4.512	-3.127
χ (eV)	3.453	4.625	2.850	3.531	5.141	2.943	3.706	4.388	3.263	3.642	4.512	3.127
ω	4.423	9.612	2.926	4.554	11.908	3.168	4.952	6.003	3.641	3.626	5.017	2.580
ω^+	2.865	7.438	1.675	2.960	9.477	1.868	3.272	4.009	2.193	2.034	3.014	1.253
ω^-	6.318	12.063	4.524	6.490	14.617	4.810	6.978	8.397	5.456	5.675	7.526	4.380
ε	0.226	0.104	0.342	0.220	0.084	0.316	0.202	0.167	0.275	0.276	0.199	0.388
ΔE back donation	-0.337	-0.278	-0.347	-0.342	-0.277	-0.342	-0.347	-0.401	-0.366	-0.457	-0.507	-0.474
ΔN_{max} (e)	-0.083	-0.627	0.137	-0.110	-0.861	0.105	-0.171	-0.361	-0.011	-0.113	-0.316	0.027

Table B6 (continued)

	Protocatechuic acid			Quercetin			Syringic acid			Vanillic acid		
	Neutral	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**
E_{HOMO} (eV)	-5.157	-6.645	-4.78	-4.881	-5.475	-4.224	-4.943	-5.713	-4.371	-5.17	-6.518	-4.612
E_{LUMO} (eV)	-1.841	-3.814	-1.284	-2.16	-2.86	-1.436	-1.825	-2.461	-1.113	-1.837	-3.796	-1.194
Dipole moment (Debye)	4.871	4.938	3.346	6.280	18.675	3.985	4.007	11.038	2.944	5.376	4.533	4.090
Molecular area ($Å^2$)	169.864	174.715		287.706	293.393		216.371	219.375		188.582	194.988	
ΔE (eV)	3.316	2.831	3.496	2.721	2.615	2.788	3.118	3.252	3.258	3.333	2.722	3.418
η (eV)	1.658	1.416	1.748	1.361	1.308	1.394	1.559	1.626	1.629	1.667	1.361	1.709
σ $(eV)^{-1}$	0.603	0.706	0.572	0.735	0.765	0.717	0.641	0.615	0.614	0.600	0.735	0.585
Pi (eV)	-3.499	-5.230	-3.032	-3.521	-4.168	-2.830	-3.384	-4.087	-2.742	-3.504	-5.157	-2.903
χ (eV)	3.499	5.230	3.032	3.521	4.168	2.830	3.384	4.087	2.742	3.504	5.157	2.903
ω	3.692	9.660	2.630	4.555	6.642	2.873	3.673	5.136	2.308	3.683	9.770	2.466
ω^+	2.150	7.222	1.332	2.965	4.721	1.632	2.176	3.296	1.140	2.139	7.362	1.228
ω^-	5.649	12.452	4.364	6.485	8.889	4.462	5.560	7.383	3.882	5.643	12.519	4.131
ε	0.271	0.104	0.380	0.220	0.151	0.348	0.272	0.195	0.433	0.272	0.102	0.406
ΔE back donation	-0.415	-0.354	-0.437	-0.340	-0.327	-0.349	-0.390	-0.407	-0.407	-0.417	-0.340	-0.427
ΔN_{max} (e)	-0.081	-0.706	0.057	-0.107	-0.359	0.143	-0.049	-0.264	0.150	-0.082	-0.708	0.096

Table B7: The quantum data for green pea peel extract in the neutral, protonated, and vacuum form*

	Naringenin			Epigallocatechin			Apigenin			Melitidin		
	Neutral	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**
E_{HOMO} (eV)	-5.086	-5.675	-4.305	-4.910	-5.691	-4.430	-5.046	-6.031	-4.182	-5.182	-6.187	-4.347
E_{LUMO} (eV)	-1.934	-2.669	-1.201	-0.779	-2.348	-0.351	-2.192	-3.565	-1.585	-2.261	-3.749	-1.352
Dipole moment (Debye)	4.775	16.487	3.711	2.415	17.982	1.576	7.970	17.089	5.047	9.410	11.976	8.287
Molecular area ($Å^2$)	276.030	281.878		294.274	304.191		271.472	273.973		648.590	648.833	
ΔE (eV)	3.152	3.006	3.104	4.131	3.343	4.079	2.854	2.466	2.597	2.921	2.438	2.995
η (eV)	1.576	1.503	1.552	2.066	1.672	2.040	1.427	1.233	1.299	1.461	1.219	1.498
$\sigma (eV)^{-1}$	0.635	0.665	0.644	0.484	0.598	0.490	0.701	0.811	0.770	0.685	0.820	0.668
Pi (eV)	-3.510	-4.172	-2.753	-2.845	-4.020	-2.391	-3.619	-4.798	-2.884	-3.722	-4.968	-2.850
χ (eV)	3.510	4.172	2.753	2.845	4.020	2.391	3.619	4.798	2.884	3.722	4.968	2.850
ω	3.909	5.790	2.442	1.959	4.833	1.401	4.589	9.335	3.202	4.741	10.123	2.711
ω^+	2.351	3.892	1.259	0.795	3.032	0.461	2.958	7.090	1.922	3.063	7.792	1.474
ω^-	5.861	8.064	4.012	3.639	7.052	2.851	6.577	11.888	4.806	6.785	12.760	4.323
ε	0.256	0.173	0.410	0.511	0.207	0.714	0.218	0.107	0.312	0.211	0.099	0.369
ΔE back donation	-0.394	-0.376	-0.388	-0.516	-0.418	-0.510	-0.357	-0.308	-0.325	-0.365	-0.305	-0.374
ΔN_{max} (e)	-0.089	-0.313	0.154	0.093	-0.236	0.206	-0.136	-0.636	0.133	-0.168	-0.713	0.127

Table B7 (continued)

	Quinic acid			2,2'-methylenebis			quercetin triglucoside		
	Neutral	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**	**Neutral**	**Protonated**	**Vacuum**
E_{HOMO} (eV)	-5.913	-8.025	-5.318	-4.752	-4.921	-4.167	-4.893	-5.850	-4.388
E_{LUMO} (eV)	-1.098	-3.734	-0.580	-0.651	-1.301	-0.107	-2.175	-3.086	-1.678
Dipole moment (Debye)	6.802	8.157	4.526	3.752	11.414	3.318	13.767	24.168	6.497
Molecular area ($Å^2$)	191.819	201.583		383.468	390.479		658.181	666.915	
ΔE (eV)	4.815	4.291	4.738	4.101	3.620	4.060	2.718	2.764	2.710
η (eV)	2.408	2.146	2.369	2.051	1.810	2.030	1.359	1.382	1.355
σ $(eV)^{-1}$	0.415	0.466	0.422	0.488	0.552	0.493	0.736	0.724	0.738
Pi (eV)	-3.506	-5.880	-2.949	-2.702	-3.111	-2.137	-3.534	-4.468	-3.033
χ (eV)	3.506	5.880	2.949	2.702	3.111	2.137	3.534	4.468	3.033
ω	2.552	8.056	1.836	1.780	2.674	1.125	4.595	7.223	3.394
ω^+	1.100	5.384	0.657	0.685	1.344	0.310	2.998	5.161	2.047
ω^-	4.606	11.264	3.606	3.387	4.455	2.447	6.532	9.629	5.080
ε	0.392	0.124	0.545	0.562	0.374	0.889	0.218	0.138	0.295
ΔE back donation	-0.602	-0.536	-0.592	-0.513	-0.453	-0.508	-0.340	-0.346	-0.339
ΔN_{max} (e)	-0.057	-0.617	0.059	0.129	0.033	0.269	-0.112	-0.448	0.073

* Excluding the compounds that are already calculated in Table B.6, such as (+)-catechin, quercetin, kaempferol, p-OH-benzoic acid, protocatechuic acid, and caffeic acid.

Table B8: Calculated Mullikan charge on the atoms of the investigated neutral, protonated, and vacuum inhibitor molecules of SCS and GPP

(+)- Catechin				Caffeic acid			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.163	0.164	0.17	C (1)	0.533	0.483	0.523
C (2)	0.226	0.226	0.232	C (2)	-0.134	-0.085	-0.121
C (3)	-0.075	-0.088	-0.067	C (3)	0.011	0.056	0.02
C (4)	-0.056	0	-0.05	O (4)	-0.545	-0.218	-0.471
C (5)	0.318	0.279	0.328	O (5)	-0.46	-0.411	-0.445
C (6)	-0.189	-0.138	-0.184	C (6)	0.102	0.122	0.121
C (7)	0.339	0.35	0.349	C (7)	-0.116	-0.078	-0.112
C (8)	-0.185	-0.141	-0.155	C (8)	0.288	0.345	0.289
C (9)	0.343	0.355	0.351	C (9)	0.289	0.293	0.294
O (10)	-0.539	-0.521	-0.514	C (10)	-0.085	-0.041	-0.069
O (11)	-0.541	-0.53	-0.5	C (11)	-0.089	-0.058	-0.071
O (12)	-0.5	-0.29	-0.47	O (12)	-0.485	-0.264	-0.457
O (13)	-0.502	-0.478	-0.464	O (13)	-0.504	-0.473	-0.492
C (14)	0.041	0.039	0.042	H (14)	0.041	0.117	0.021
C (15)	-0.129	-0.079	-0.106	H (15)	0.041	0.098	0.036
C (16)	0.291	0.269	0.305	H (16)	0.282	0.33	0.247
C (17)	0.276	0.331	0.28	H (17)	0.05	0.324	0.011
C (18)	-0.108	-0.087	-0.098	H (18)	0.047	0.09	0.029
C (19)	-0.066	-0.024	-0.053	H (19)	0.041	0.098	0.017
O (20)	-0.507	-0.483	-0.493	H (20)	0.299	0.08	0.274
O (21)	-0.505	-0.277	-0.47	H (21)	0.294	0.39	0.255
H (22)	0.044	0.066	0.028	H (22)		0.384	
H (23)	0.041	0.056	0.022	H (23)		0.317	
H (24)	0.056	0.078	0.053				
H (25)	0.055	0.079	0.051				
H (26)	0.049	0.084	-0.007				
H (27)	0.035	0.06	0.031				
H (28)	0.264	0.274	0.235				
H (29)	0.284	0.378	0.242				
H (30)	0.285	0.376	0.241				
H (31)	0.039	0.294	0.038				
H (32)	0.042	0.083	0.002				
H (33)	0.03	0.069	0.01				
H (34)	0.292	0.056	0.251				
H (35)	0.294	0.311	0.269				
H (36)		0.377					
H (37)		0.382					

Table B8 (continued)

Chlorogenic acid				Ferulic acid			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.128	0.132	0.128	C (1)	0.533	0.541	0.523
C (2)	-0.037	-0.063	-0.028	C (2)	-0.136	-0.112	-0.123
C (3)	0.193	0.21	0.184	C (3)	0.015	0.021	0.025
C (4)	0.208	0.168	0.212	O (4)	-0.543	-0.517	-0.467
C (5)	0.229	0.211	0.224	O (5)	-0.46	-0.446	-0.446
C (6)	-0.052	-0.057	-0.045	C (6)	0.102	0.125	0.121
C (7)	0.592	0.509	0.564	C (7)	-0.089	-0.078	-0.078
O (8)	-0.481	-0.129	-0.437	C (8)	0.28	0.334	0.291
O (9)	-0.414	-0.373	-0.417	C (9)	0.295	0.247	0.29
O (10)	-0.546	-0.524	-0.484	C (10)	-0.09	-0.041	-0.083
O (11)	-0.534	-0.51	-0.489	C (11)	-0.082	-0.069	-0.07
O (12)	-0.532	-0.434	-0.491	O (12)	-0.581	-0.559	-0.541
O (13)	-0.519	-0.45	-0.522	C (13)	0.201	0.188	0.208
C (14)	0.567	0.625	0.556	O (14)	-0.474	-0.282	-0.454
C (15)	-0.143	-0.109	-0.135	H (15)	0.041	0.055	0.018
C (16)	0.013	0.047	0.023	H (16)	0.042	0.056	0.041
O (17)	-0.529	-0.435	-0.465	H (17)	0.283	0.29	0.247
C (18)	0.1	0.099	0.118	H (18)	0.043	0.065	0.027
C (19)	-0.118	-0.059	-0.136	H (19)	0.053	0.084	0.009
C (20)	0.276	0.263	0.293	H (20)	0.044	0.064	0.016
C (21)	0.298	0.345	0.297	H (21)	0.036	0.054	0.018
C (22)	-0.09	-0.062	-0.075	H (22)	0.046	0.054	0.046
C (23)	-0.052	-0.009	-0.046	H (23)	0.047	0.064	0.033
O (24)	-0.48	-0.431	-0.455	H (24)	0.294	0.382	0.249
O (25)	-0.537	-0.292	-0.492	H (25)		0.381	
H (26)	0.055	0.114	0.034				
H (27)	0.066	0.119	0.069				
H (28)	0.08	0.119	0.082				
H (29)	0.046	0.106	0.039				
H (30)	0.061	0.094	0.04				
H (31)	0.05	0.094	0.019				
H (32)	0.065	0.103	0.085				
H (33)	0.306	0.348	0.266				
H (34)	0.277	0.344	0.234				
H (35)	0.277	0.293	0.249				
H (36)	0.276	0.327	0.26				
H (37)	0.039	0.371	0.012				
H (38)	0.043	0.307	0.042				
H (39)	0.048	0.077	0.011				
H (40)	0.047	0.087	0.029				
H (41)	0.04	0.098	0.016				
H (42)	0.287	0.079	0.275				
H (43)	0.3	0.071	0.256				
H (44)		0.304					
H (45)		0.385					
H (46)		0.387					

Table B8 (continued)

Gallic acid				Kaempferol			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.521	0.514	0.51	C (1)	0.272	0.311	0.252
C (2)	0.004	0.043	0.011	C (2)	0.218	0.274	0.218
C (3)	-0.134	-0.096	-0.114	C (3)	0.311	0.356	0.313
C (4)	0.304	0.369	0.31	C (4)	-0.055	-0.004	-0.055
C (5)	0.243	0.223	0.241	C (5)	0.313	0.351	0.323
C (6)	0.298	0.364	0.298	C (6)	-0.167	-0.138	-0.173
C (7)	-0.137	-0.1	-0.132	C (7)	0.349	0.361	0.352
O (8)	-0.527	-0.254	-0.455	C (8)	-0.172	-0.148	-0.157
O (9)	-0.459	-0.332	-0.456	C (9)	0.324	0.343	0.327
O (10)	-0.505	-0.452	-0.498	O (10)	-0.495	-0.45	-0.498
O (11)	-0.496	-0.288	-0.491	O (11)	-0.577	-0.423	-0.453
O (12)	-0.499	-0.44	-0.466	C (12)	0.012	0.033	0.024
H (13)	0.047	0.097	0.054	C (13)	-0.041	-0.014	-0.027
H (14)	0.059	0.109	0.033	C (14)	-0.084	-0.044	-0.079
H (15)	0.285	0.359	0.249	C (15)	0.338	0.338	0.34
H (16)	0.295	0.362	0.255	C (16)	-0.079	-0.042	-0.063
H (17)	0.304	0.317	0.279	C (17)	-0.076	-0.058	-0.077
H (18)	0.297	0.394	0.27	O (18)	-0.484	-0.258	-0.453
H (19)		0.393		O (19)	-0.48	-0.445	-0.455
H (20)		0.319		O (20)	-0.469	-0.489	-0.416
				O (21)	-0.504	-0.475	-0.454
				H (22)	0.062	0.086	0.001
				H (23)	0.052	0.076	0.033
				H (24)	0.046	0.079	0.028
				H (25)	0.05	0.095	0.01
				H (26)	0.047	0.097	0.03
				H (27)	0.049	0.082	0.036
				H (28)	0.29	0.38	0.247
				H (29)	0.292	0.381	0.247
				H (30)	0.287	0.303	0.241
				H (31)	0.273	0.332	0.239
				H (32)		0.317	
				H (33)		0.295	

Table B8 (continued)

Myricetin				p- coumaric acid			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.259	0.359	0.249	C (1)	0.532	0.54	0.522
C (2)	0.229	0.266	0.222	C (2)	-0.134	-0.11	-0.114
C (3)	0.312	0.377	0.314	C (3)	0.011	0.016	0.017
C (4)	-0.053	0.021	-0.055	O (4)	-0.537	-0.514	-0.456
C (5)	0.314	0.349	0.324	O (5)	-0.471	-0.457	-0.46
C (6)	-0.166	-0.094	-0.173	C (6)	0.098	0.117	0.116
C (7)	0.349	0.332	0.353	C (7)	-0.07	-0.056	-0.055
C (8)	-0.171	-0.095	-0.156	C (8)	-0.091	-0.058	-0.085
C (9)	0.324	0.349	0.328	C (9)	0.337	0.322	0.34
O (10)	-0.492	-0.445	-0.495	C (10)	-0.09	-0.06	-0.071
O (11)	-0.572	-0.382	-0.449	C (11)	-0.041	-0.032	-0.029
C (12)	0.034	0.053	0.05	O (12)	-0.48	-0.262	-0.451
C (13)	-0.13	-0.096	-0.115	H (13)	0.036	0.05	0.021
C (14)	0.318	0.334	0.322	H (14)	0.051	0.063	0.039
C (15)	0.213	0.233	0.177	H (15)	0.282	0.288	0.247
C (16)	0.318	0.341	0.319	H (16)	0.043	0.065	0.019
C (17)	-0.17	-0.117	-0.177	H (17)	0.05	0.086	0.01
O (18)	-0.49	-0.452	-0.461	H (18)	0.044	0.086	0.027
O (19)	-0.548	-0.28	-0.535	H (19)	0.04	0.064	0.015
O (20)	-0.491	-0.478	-0.462	H (20)	0.29	0.375	0.247
O (21)	-0.479	-0.269	-0.453	H (21)		0.379	
O (22)	-0.468	-0.425	-0.416				
O (23)	-0.501	-0.52	-0.45				
H (24)	0.063	0.112	0.002				
H (25)	0.053	0.111	0.036				
H (26)	0.047	0.089	0.04				
H (27)	0.053	0.099	0.048				
H (28)	0.292	0.302	0.26				
H (29)	0.311	0.376	0.269				
H (30)	0.291	0.393	0.259				
H (31)	0.292	0.317	0.247				
H (32)	0.287	0.383	0.241				
H (33)	0.271	0.391	0.239				
H (34)		0.312					
H (35)		0.328					
H (36)		0.325					

Table B8 (continued)

p-OH benzoic acid				protocatechuic acid			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.523	0.539	0.512	C (1)	0.521	0.5	0.51
C (2)	-0.003	0.018	0.006	C (2)	-0.002	0.036	0.007
C (3)	-0.043	-0.025	-0.031	C (3)	-0.116	-0.071	-0.109
C (4)	-0.086	-0.053	-0.082	C (4)	0.298	0.353	0.293
C (5)	0.341	0.333	0.344	C (5)	0.295	0.315	0.303
C (6)	-0.081	-0.054	-0.065	C (6)	-0.082	-0.031	-0.069
C (7)	-0.041	-0.027	-0.025	C (7)	-0.062	-0.025	-0.044
O (8)	-0.531	-0.498	-0.462	O (8)	-0.529	-0.25	-0.459
O (9)	-0.459	-0.441	-0.452	O (9)	-0.461	-0.34	-0.457
O (10)	-0.48	-0.261	-0.451	O (10)	-0.484	-0.255	-0.458
H (11)	0.044	0.07	0.041	O (11)	-0.504	-0.463	-0.501
H (12)	0.049	0.087	0.007	H (12)	0.061	0.11	0.036
H (13)	0.044	0.087	0.024	H (13)	0.046	0.107	0.027
H (14)	0.051	0.076	0.041	H (14)	0.042	0.095	0.042
H (15)	0.284	0.293	0.248	H (15)	0.284	0.358	0.249
H (16)	0.29	0.377	0.246	H (16)	0.299	0.362	0.273
H (17)		0.378		H (17)	0.294	0.39	0.257
				H (18)		0.388	
				H (19)		0.32	

Table B8 (continued)

Quercetin				syringic acid			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.264	0.281	0.244	C (1)	0.518	0.534	0.507
C (2)	0.226	0.242	0.224	C (2)	0.006	0.023	0.013
C (3)	0.312	0.326	0.313	C (3)	-0.157	-0.143	-0.148
C (4)	-0.054	-0.03	-0.056	C (4)	0.324	0.378	0.324
C (5)	0.314	0.33	0.322	C (5)	0.232	0.198	0.232
C (6)	-0.166	-0.117	-0.173	C (6)	0.318	0.364	0.32
C (7)	0.349	0.318	0.353	C (7)	-0.124	-0.11	-0.106
C (8)	-0.171	-0.112	-0.157	O (8)	-0.53	-0.497	-0.469
C (9)	0.325	0.333	0.327	O (9)	-0.46	-0.439	-0.448
O (10)	-0.493	-0.477	-0.494	O (10)	-0.564	-0.524	-0.536
O (11)	-0.573	-0.531	-0.453	C (11)	0.204	0.161	0.214
O (12)	-0.479	-0.277	-0.454	O (12)	-0.57	-0.574	-0.569
O (13)	-0.468	-0.442	-0.416	C (13)	0.188	0.186	0.202
O (14)	-0.501	-0.48	-0.454	O (14)	-0.489	-0.301	-0.482
C (15)	0.028	0.051	0.031	H (15)	0.055	0.077	0.047
C (16)	-0.105	-0.087	-0.089	H (16)	0.051	0.075	0.05
C (17)	0.309	0.349	0.309	H (17)	0.284	0.294	0.248
C (18)	0.275	0.242	0.284	H (18)	0.05	0.076	0.037
C (19)	-0.063	-0.03	-0.082	H (19)	0.048	0.075	0.03
C (20)	-0.102	-0.096	-0.102	H (20)	0.05	0.066	0.042
O (21)	-0.538	-0.291	-0.486	H (21)	0.055	0.073	0.041
O (22)	-0.491	-0.455	-0.462	H (22)	0.055	0.069	0.041
H (23)	0.063	0.095	0.001	H (23)	0.058	0.073	0.037
H (24)	0.052	0.092	0.035	H (24)	0.298	0.379	0.276
H (25)	0.293	0.38	0.246	H (25)		0.387	
H (26)	0.287	0.384	0.24				
H (27)	0.271	0.298	0.237				
H (28)	0.05	0.281	0.04				
H (29)	0.049	0.076	0.012				
H (30)	0.047	0.089	0.032				
H (31)	0.303	0.072	0.255				
H (32)	0.287	0.386	0.272				
H (33)		0.388					
H (34)		0.311					

Table B8 (continued)

vanillic acid				Apigenin			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.52	0.499	0.507	C (1)	0.355	0.383	0.352
C (2)	-0.002	0.038	0.008	C (2)	-0.173	-0.124	-0.157
C (3)	-0.123	-0.096	-0.128	C (3)	0.34	0.39	0.34
C (4)	0.31	0.387	0.318	C (4)	-0.054	-0.002	-0.051
C (5)	0.3	0.311	0.303	C (5)	0.313	0.355	0.323
C (6)	-0.085	-0.029	-0.072	C (6)	-0.167	-0.133	-0.173
C (7)	-0.057	-0.026	-0.046	C (7)	0.349	0.362	0.353
O (8)	-0.53	-0.246	-0.461	C (8)	-0.172	-0.151	-0.158
O (9)	-0.46	-0.341	-0.458	C (9)	0.329	0.348	0.335
O (10)	-0.576	-0.548	-0.561	O (10)	-0.503	-0.461	-0.509
C (11)	0.189	0.177	0.2	O (11)	-0.593	-0.43	-0.475
O (12)	-0.485	-0.264	-0.46	C (12)	0.046	0.071	0.06
H (13)	0.065	0.111	0.047	C (13)	-0.051	-0.023	-0.037
H (14)	0.046	0.106	0.026	C (14)	-0.089	-0.045	-0.085
H (15)	0.043	0.095	0.041	C (15)	0.336	0.335	0.339
H (16)	0.285	0.357	0.248	C (16)	-0.089	-0.053	-0.073
H (17)	0.048	0.354	0.038	C (17)	-0.068	-0.048	-0.054
H (18)	0.056	0.078	0.038	O (18)	-0.482	-0.26	-0.453
H (19)	0.057	0.08	0.039	O (19)	-0.479	-0.444	-0.454
H (20)	0.297	0.078	0.273	O (20)	-0.47	-0.494	-0.417
H (21)		0.391		H (21)	0.043	0.093	0.029
H (22)		0.388		H (22)	0.062	0.082	0.001
				H (23)	0.054	0.084	0.033
				H (24)	0.054	0.085	0.038
				H (25)	0.049	0.093	0.007
				H (26)	0.046	0.096	0.029
				H (27)	0.046	0.079	0.022
				H (28)	0.29	0.376	0.247
				H (29)	0.292	0.385	0.247
				H (30)	0.287	0.303	0.24
				H (31)		0.329	
				H (32)		0.318	

Table B8 (continued)

Quinic acid				2,2'-methylenebis			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.135	0.14	0.136	C (1)	-0.129	-0.118	-0.119
C (2)	-0.05	-0.073	-0.04	C (2)	0.271	0.273	0.278
C (3)	0.204	0.179	0.192	C (3)	-0.01	0.025	-0.015
C (4)	0.204	0.193	0.198	C (4)	-0.101	-0.101	-0.088
C (5)	0.225	0.173	0.229	C (5)	0.043	0.044	0.061
C (6)	-0.029	-0.07	-0.022	C (6)	-0.091	-0.083	-0.077
C (7)	0.551	0.499	0.536	C (7)	0.033	0.034	0.036
O (8)	-0.492	-0.163	-0.44	C (8)	-0.128	-0.129	-0.129
O (9)	-0.442	-0.351	-0.448	C (9)	-0.053	-0.053	-0.041
O (10)	-0.548	-0.248	-0.489	C (10)	-0.049	-0.05	-0.036
O (11)	-0.541	-0.497	-0.488	C (11)	-0.058	-0.059	-0.045
O (12)	-0.54	-0.259	-0.5	C (12)	-0.104	-0.105	-0.093
O (13)	-0.524	-0.445	-0.484	O (13)	-0.52	-0.519	-0.493
H (14)	0.06	0.13	0.04	C (14)	0.275	0.259	0.294
H (15)	0.055	0.131	0.06	C (15)	0.007	0.013	0.014
H (16)	0.051	0.15	0.033	C (16)	-0.093	-0.076	-0.072
H (17)	0.035	0.132	-0.006	C (17)	0.044	0.072	0.063
H (18)	0.051	0.151	0.043	C (18)	-0.096	-0.092	-0.072
H (19)	0.048	0.129	0.046	C (19)	0.034	0.065	0.04
H (20)	0.056	0.135	0.072	C (20)	-0.108	-0.125	-0.097
H (21)	0.293	0.36	0.258	C (21)	-0.045	-0.038	-0.045
H (22)	0.272	0.359	0.233	C (22)	-0.028	-0.032	-0.027
H (23)	0.272	0.378	0.251	C (23)	-0.036	-0.15	-0.034
H (24)	0.28	0.382	0.241	C (24)	-0.103	-0.106	-0.094
H (25)	0.275	0.322	0.25	O (25)	-0.517	-0.323	-0.498
H (26)		0.37		H (26)	0.064	0.063	0.064
H (27)		0.383		H (27)	0.054	0.077	0.042
H (28)		0.311		H (28)	0.022	0.025	0.019
				H (29)	0.028	0.032	0.005
				H (30)	0.035	0.036	0.022
				H (31)	0.03	0.03	0.018
				H (32)	0.035	0.035	0.034
				H (33)	0.033	0.035	0.018
				H (34)	0.032	0.034	0.031
				H (35)	0.029	0.03	0.022
				H (36)	0.033	0.034	0.028
				H (37)	0.029	0.03	0.016
				H (38)	0.032	0.034	0.027
				H (39)	0.032	0.034	0.025
				H (40)	0.043	0.045	0.033
				H (41)	0.036	0.038	0.022
				H (42)	0.274	0.274	0.246
				H (43)	0.018	0.041	-0.003
				H (44)	0.031	0.055	0.007
				H (45)	0.021	0.037	0.02
				H (46)	0.029	0.038	0.019
				H (47)	0.023	0.04	0.014
				H (48)	0.02	0.038	0.011
				H (49)	0.022	0.038	0.042
				H (50)	0.021	0.036	0.007
				H (51)	0.03	0.073	0.051
				H (52)	0.017	0.073	0.014
				H (53)	0.018	0.072	0.006
				H (54)	0.032	0.043	0.019
				H (55)	0.042	0.057	0.032
				H (56)	0.035	0.047	0.025
				H (57)	0.263	0.365	0.251
				H (58)		0.336	

Table B8 (continued)

quercetin triglucoside				Melitidin			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
C (1)	0.308	0.348	0.319	C (1)	0.541	0.536	0.546
C (2)	0.192	0.201	0.195	C (2)	-0.096	-0.125	-0.106
C (3)	0.316	0.33	0.31	C (3)	0.189	0.201	0.207
C (4)	-0.049	-0.021	-0.048	C (4)	-0.096	-0.104	-0.1
C (5)	0.316	0.332	0.323	C (5)	0.57	0.578	0.593
C (6)	-0.166	-0.116	-0.173	O (6)	-0.478	-0.098	-0.445
C (7)	0.348	0.325	0.354	O (7)	-0.438	-0.454	-0.413
C (8)	-0.172	-0.117	-0.159	O (8)	-0.487	-0.484	-0.465
C (9)	0.326	0.341	0.332	C (9)	-0.072	-0.096	-0.062
O (10)	-0.496	-0.489	-0.501	O (10)	-0.526	-0.5	-0.503
O (11)	-0.568	-0.528	-0.493	O (11)	-0.486	-0.457	-0.462
O (12)	-0.478	-0.273	-0.45	C (12)	0.212	0.178	0.19
O (13)	-0.469	-0.441	-0.421	O (13)	-0.542	-0.528	-0.514
C (14)	0.036	0.022	0.04	C (14)	0.178	0.165	0.182
C (15)	-0.114	-0.051	-0.098	C (15)	0.22	0.156	0.226
C (16)	0.295	0.269	0.303	C (16)	0.178	0.177	0.214
C (17)	0.286	0.336	0.282	C (17)	0.242	0.237	0.213
C (18)	-0.099	-0.082	-0.092	C (18)	0.452	0.425	0.459
C (19)	-0.074	-0.05	-0.066	O (19)	-0.552	-0.52	-0.537
O (20)	-0.495	-0.458	-0.486	O (20)	-0.568	-0.528	-0.521
O (21)	-0.5	-0.277	-0.47	C (21)	0.43	0.455	0.475
O (22)	-0.552	-0.541	-0.545	C (22)	0.217	0.152	0.215
O (23)	-0.544	-0.521	-0.53	C (23)	0.227	0.209	0.203
C (24)	0.484	0.467	0.483	C (24)	0.188	0.162	0.235
C (25)	0.179	0.193	0.178	C (25)	0.19	0.177	0.222
C (26)	0.234	0.174	0.234	C (26)	-0.063	-0.089	-0.062
C (27)	0.216	0.183	0.202	O (27)	-0.541	-0.256	-0.504
C (28)	0.188	0.172	0.216	O (28)	-0.554	-0.507	-0.518
C (29)	0.223	0.204	0.219	O (29)	-0.548	-0.258	-0.513
O (30)	-0.557	-0.268	-0.515	O (30)	-0.523	-0.487	-0.507
O (31)	-0.532	-0.51	-0.531	C (31)	0.161	0.17	0.16
O (32)	-0.564	-0.268	-0.509	C (32)	-0.102	-0.134	-0.09
O (33)	-0.534	-0.528	-0.528	C (33)	0.355	0.398	0.318
O (34)	-0.551	-0.531	-0.525	C (34)	-0.055	-0.019	-0.059
C (35)	0.478	0.47	0.491	C (35)	0.33	0.369	0.325
C (36)	0.203	0.208	0.201	C (36)	-0.167	-0.139	-0.177
C (37)	0.226	0.187	0.236	C (37)	0.357	0.381	0.366
C (38)	0.208	0.187	0.216	C (38)	-0.166	-0.139	-0.146
C (39)	0.199	0.197	0.21	C (39)	0.349	0.375	0.342
O (40)	-0.545	-0.562	-0.488	O (40)	-0.527	-0.495	-0.503
O (41)	-0.545	-0.536	-0.533	O (41)	-0.575	-0.383	-0.439
C (42)	0.478	0.445	0.464	C (42)	0.041	0.081	0.069
C (43)	0.209	0.165	0.228	C (43)	-0.051	-0.032	-0.03
C (44)	0.196	0.216	0.232	C (44)	-0.086	-0.04	-0.065
C (45)	0.228	0.198	0.213	C (45)	0.337	0.307	0.343
C (46)	0.194	0.191	0.198	C (46)	-0.096	-0.041	-0.087
C (47)	0.22	0.207	0.216	C (47)	-0.038	-0.036	-0.027
O (48)	-0.559	-0.356	-0.513	O (48)	-0.494	-0.276	-0.458
O (49)	-0.537	-0.534	-0.512	O (49)	-0.515	-0.479	-0.421
O (50)	-0.539	-0.499	-0.516	O (50)	-0.521	-0.506	-0.503
O (51)	-0.539	-0.302	-0.508	O (51)	-0.529	-0.316	-0.523
C (52)	0.213	0.207	0.206	H (52)	0.087	0.172	0.06
O (53)	-0.547	-0.365	-0.511	H (53)	0.078	0.173	0.076
O (54)	-0.525	-0.536	-0.497	H (54)	0.075	0.099	0.058
O (55)	-0.535	-0.512	-0.541	H (55)	0.081	0.113	0.066
H (56)	0.064	0.099	0.003	H (56)	0.298	0.325	0.263
H (57)	0.054	0.097	0.041	H (57)	0.048	0.326	0.018

Table B8 (continued)

quercetin triglucoside				Melitidin			
	Neutral	**Protonated**	**Gas**		**Neutral**	**Protonated**	**Gas**
H (58)	0.293	0.387	0.247	H (58)	0.047	0.07	0.069
H (59)	0.288	0.379	0.242	H (59)	0.045	0.063	0.039
H (60)	0.05	0.3	0.046	H (60)	0.275	0.067	0.266
H (61)	0.053	0.1	0.014	H (61)	0.076	0.293	0.055
H (62)	0.052	0.081	0.06	H (62)	0.072	0.098	0.072
H (63)	0.296	0.081	0.257	H (63)	0.076	0.108	0.049
H (64)	0.296	0.313	0.27	H (64)	0.062	0.125	0.026
H (65)	0.051	0.381	0.046	H (65)	0.079	0.148	0.057
H (66)	0.069	0.386	0.057	H (66)	0.067	0.142	0.05
H (67)	0.062	0.091	0.033	H (67)	0.059	0.11	0.032
H (68)	0.052	0.115	0.031	H (68)	0.077	0.094	0.035
H (69)	0.047	0.15	0.009	H (69)	0.05	0.087	0.033
H (70)	0.042	0.118	0.031	H (70)	0.058	0.15	0.028
H (71)	0.048	0.108	0.077	H (71)	0.056	0.137	0.025
H (72)	0.282	0.137	0.246	H (72)	0.049	0.153	0.026
H (73)	0.277	0.133	0.269	H (73)	0.043	0.104	0.03
H (74)	0.278	0.376	0.281	H (74)	0.044	0.079	0.05
H (75)	0.047	0.379	0.032	H (75)	0.038	0.075	0.028
H (76)	0.063	0.323	0.041	H (76)	0.279	0.074	0.256
H (77)	0.051	0.369	0.034	H (77)	0.279	0.377	0.258
H (78)	0.058	0.375	0.044	H (78)	0.269	0.376	0.259
H (79)	0.049	0.079	0.026	H (79)	0.061	0.312	0.029
H (80)	0.057	0.11	0.015	H (80)	0.079	0.381	0.05
H (81)	0.036	0.101	0.042	H (81)	0.073	0.374	0.053
H (82)	0.06	0.106	0.025	H (82)	0.06	0.103	0.022
H (83)	0.053	0.093	0.034	H (83)	0.047	0.117	0.032
H (84)	0.042	0.111	0.014	H (84)	0.041	0.13	0.026
H (85)	0.044	0.149	0.036	H (85)	0.041	0.089	0.026
H (86)	0.046	0.114	0.057	H (86)	0.046	0.078	0.006
H (87)	0.281	0.113	0.247	H (87)	0.04	0.073	0.011
H (88)	0.278	0.106	0.263	H (88)	0.287	0.085	0.245
H (89)	0.281	0.127	0.262	H (89)	0.305	0.086	0.242
H (90)	0.273	0.12	0.267	H (90)	0.283	0.071	0.259
H (91)	0.046	0.362	0.031	H (91)	0.289	0.375	0.274
H (92)	0.043	0.321	0.048	H (92)		0.383	
H (93)	0.282	0.407	0.246	H (93)		0.338	
H (94)	0.272	0.309	0.253	H (94)		0.324	
H (95)	0.272	0.376	0.283	H (95)		0.327	
H (96)		0.389		H (96)		0.378	
H (97)		0.121		H (97)		0.376	
H (98)		0.116					
H (99)		0.359					
H (100)		0.32					
H (101)		0.408					
H (102)		0.3					

Table B9: The electrostatic potentials of the neutral and protonated molecules as the contour of the SCS and GPP extracts' electrostatic field

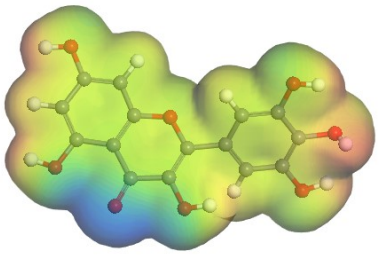
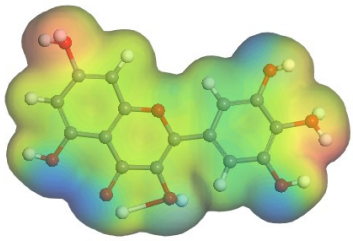
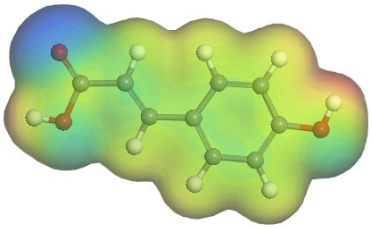
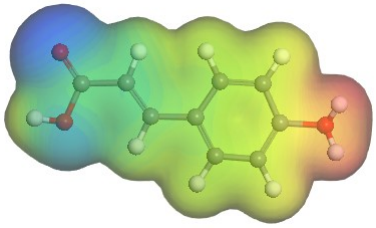
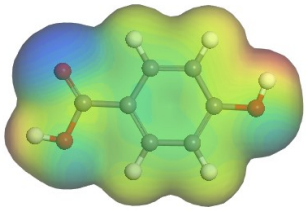
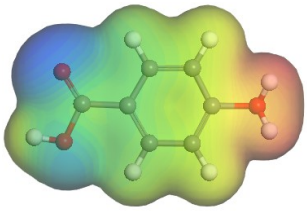
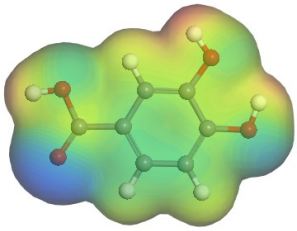
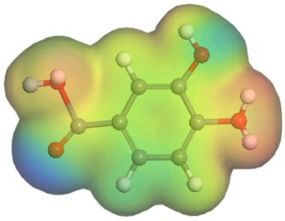
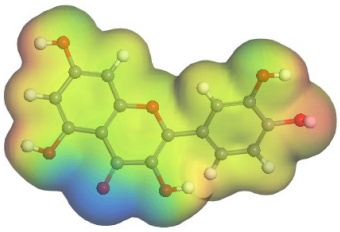
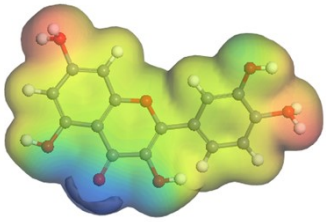
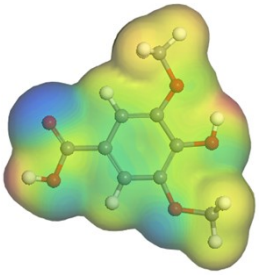
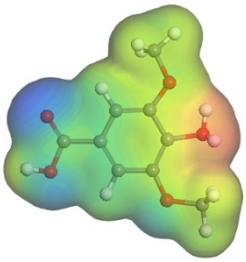
Plant	Compound	Neutral	Protonated
SCS	Myricetin		
SCS	p- coumaric acid		
SCS& GPP	p-OH benzoic acid		
SCS& GPP	Protocatechuic acid		
SCS& GPP	Quercetin		
SCS	Syringic acid		

Table B9 (continued)

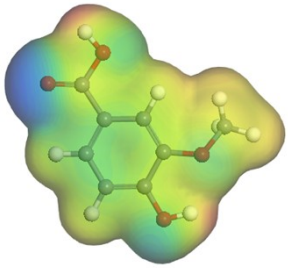
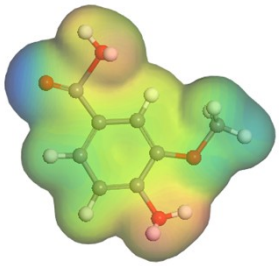
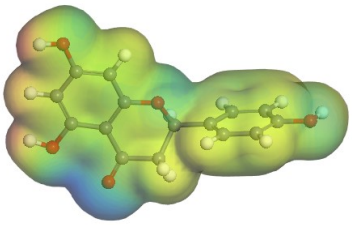
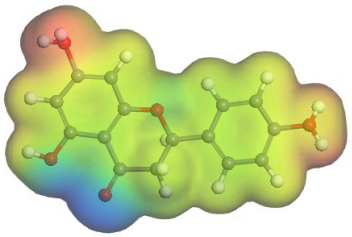
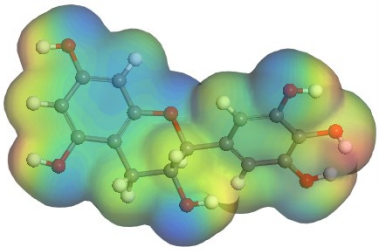
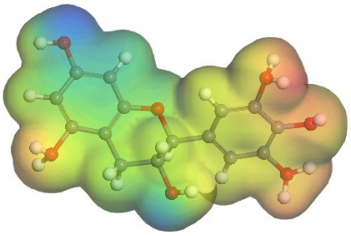
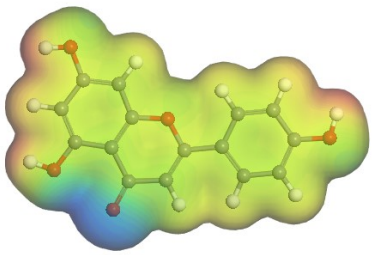
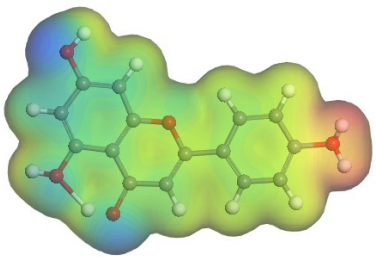
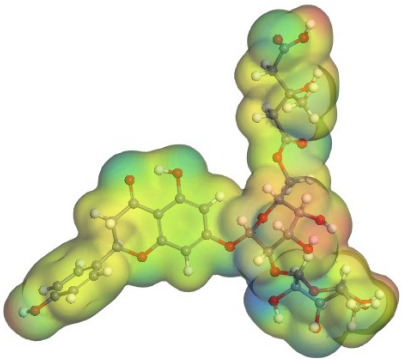
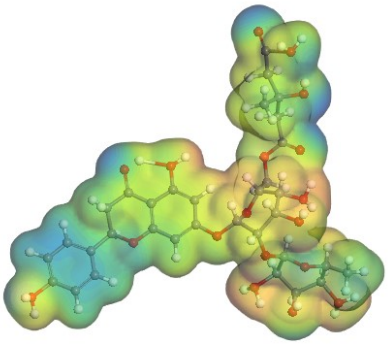
Plant	Compound	Neutral	Protonated
SCS	Vanillic acid		
GPP	Naringenin		
GPP	Epigallocatechin		
GPP	Apigenin		
GPP	Melitidin		

Table B9 (continued)

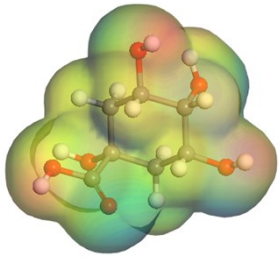
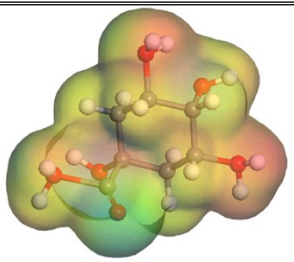
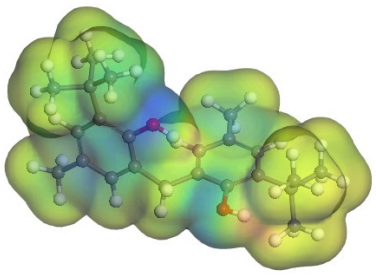
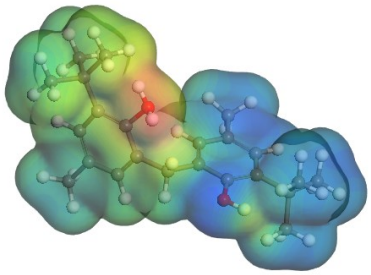
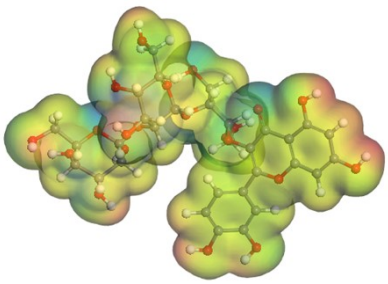
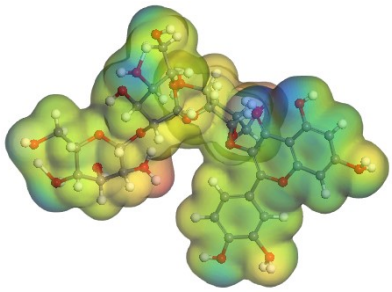
Plant	Compound	Neutral	Protonated
GPP	Quinic acid		
GPP	2,2'-methylenebis		
GPP	Quercetin triglucoside		

Table B10: The best formation for adsorption of SCS and GPP extracts on aluminum (1 1 1) substrate as determined by the adsorption locator module

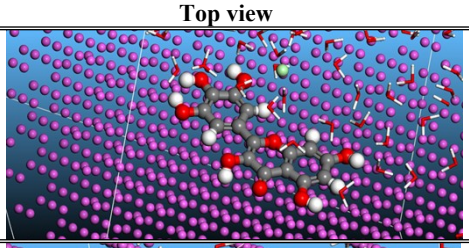
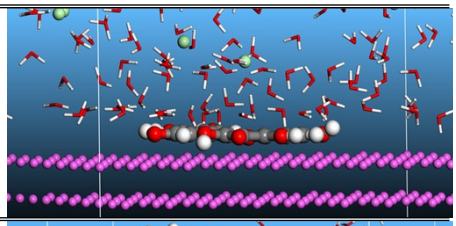
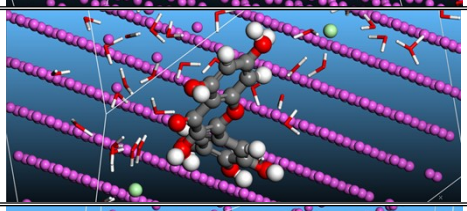
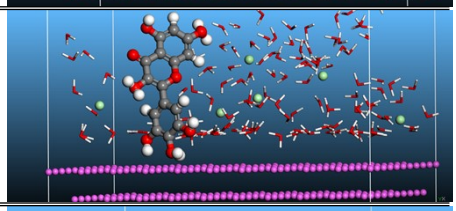
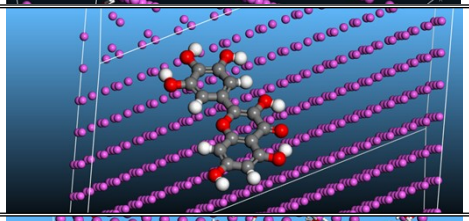
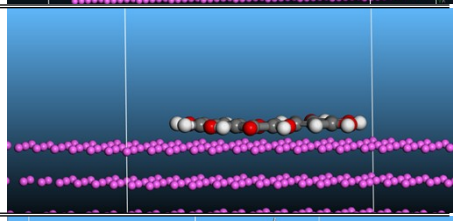
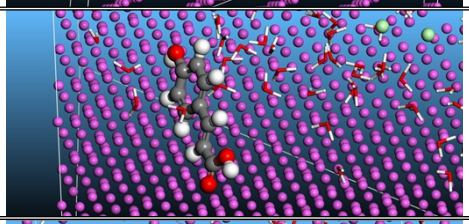
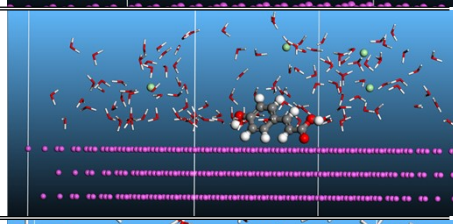
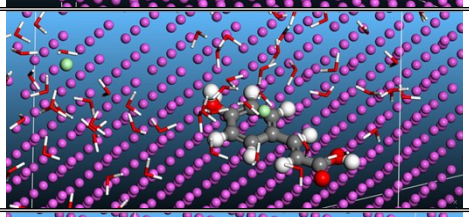
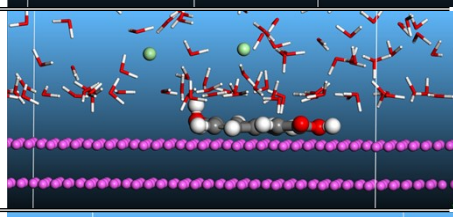
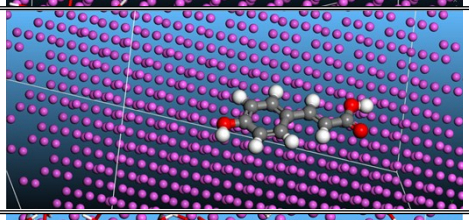
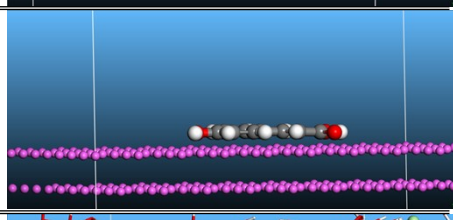
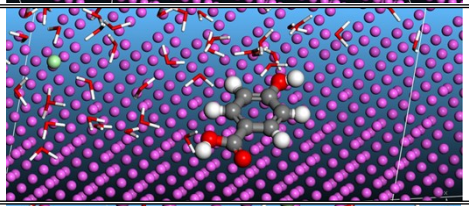
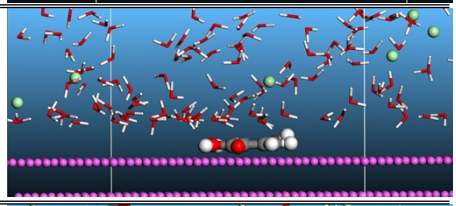
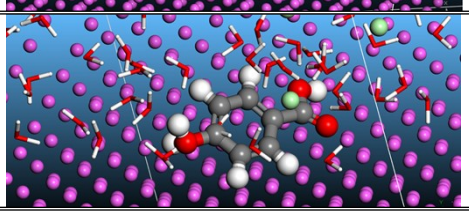
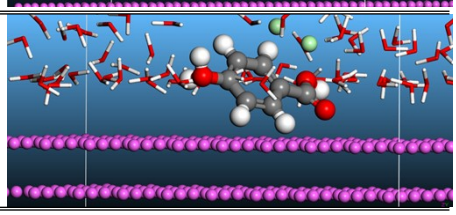
Compound		Top view	Side view
Myricetin	neutral		
	protonated		
	vacuum		
p- coumaric acid	neutral		
	protonated		
	vacuum		
p-OH benzoic acid	neutral		
	protonated		

Table B10 (continued)

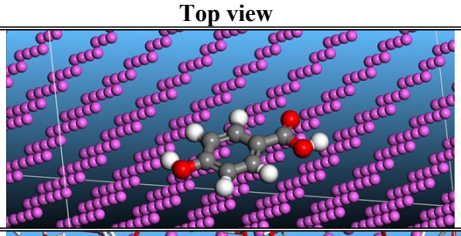
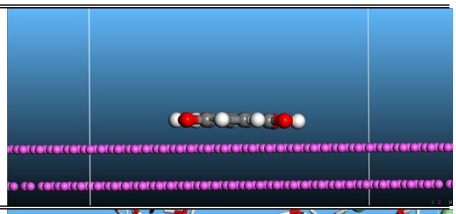
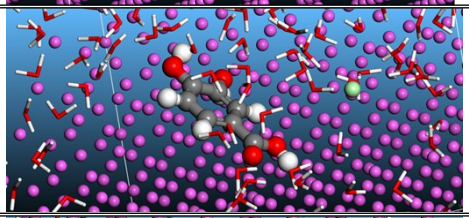
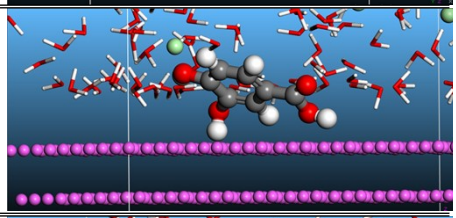
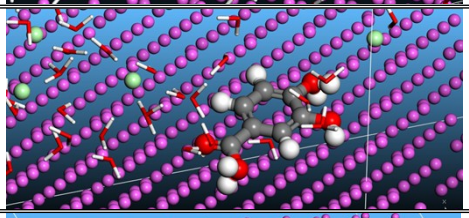
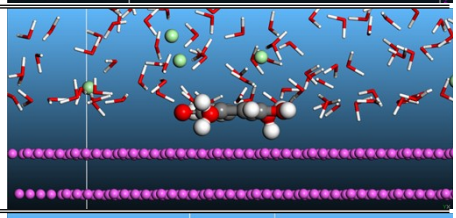
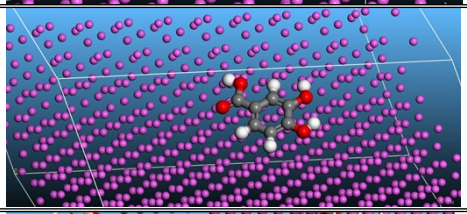
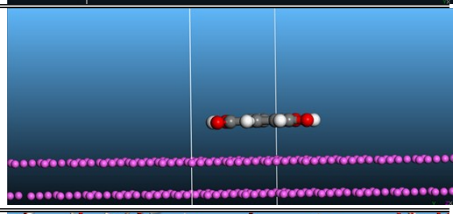
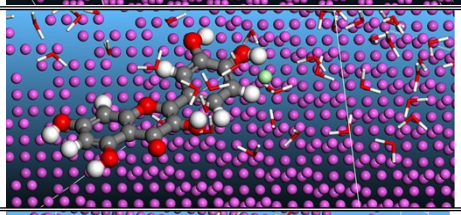
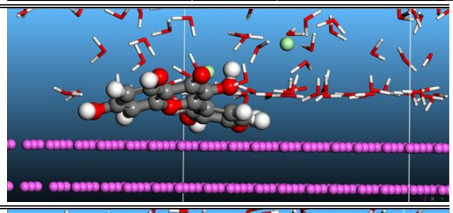
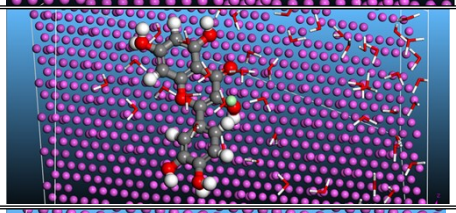
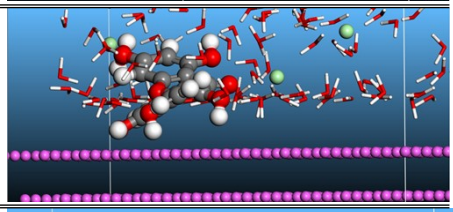
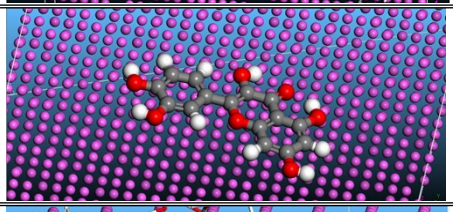
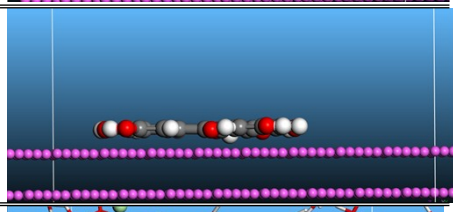
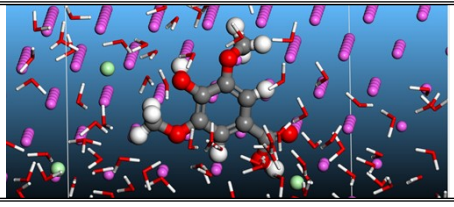
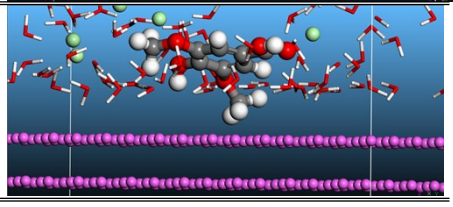
Compound		Top view	Side view
p-OH benzoic acid	vacuum		
Protocatechuic acid	neutral		
	protonated		
	vacuum		
Quercetin	neutral		
	protonated		
	vacuum		
Syringic acid	neutral		

Table B10 (continued)

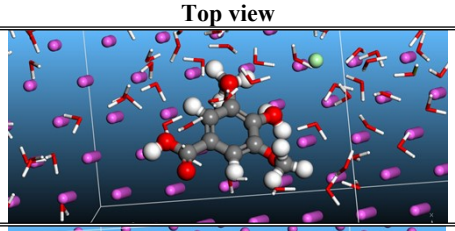
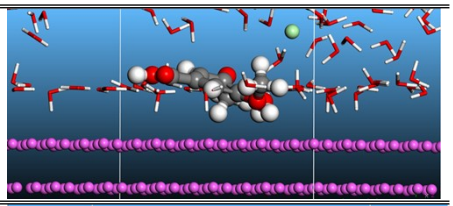
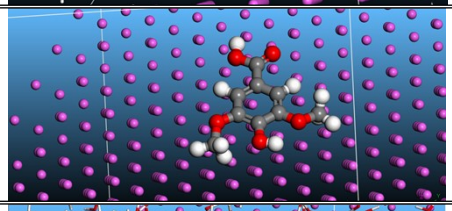
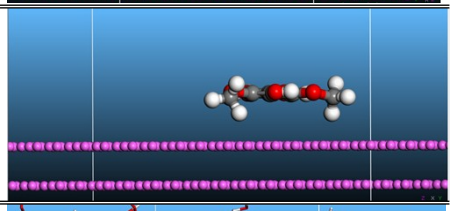
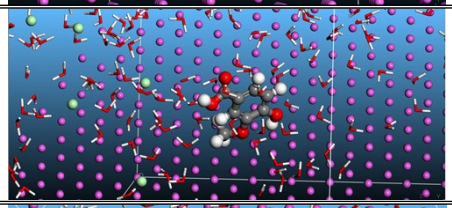
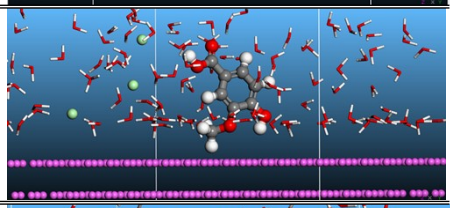
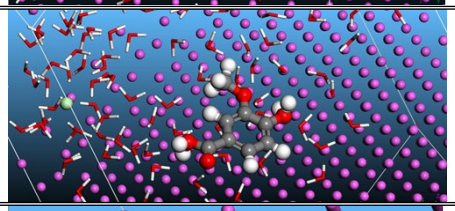
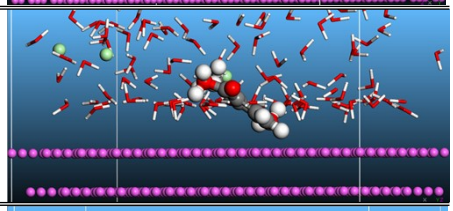
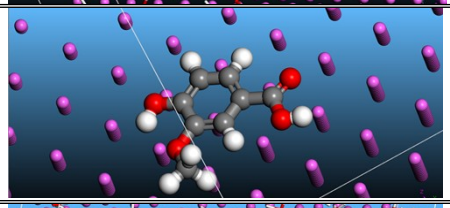
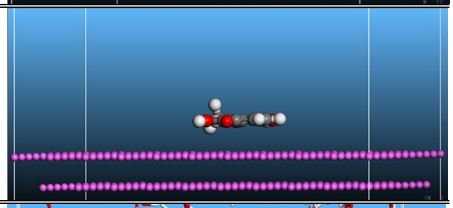
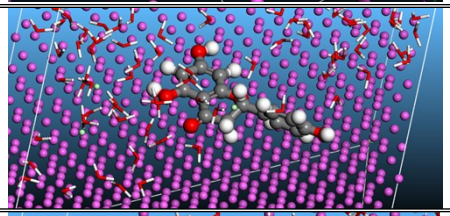
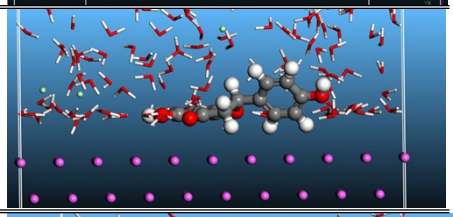
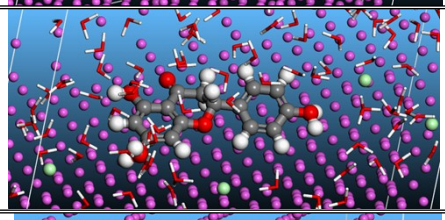
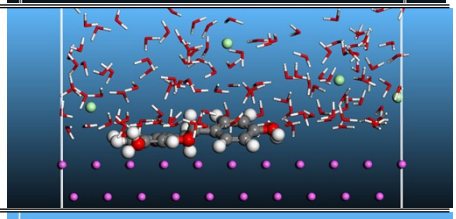
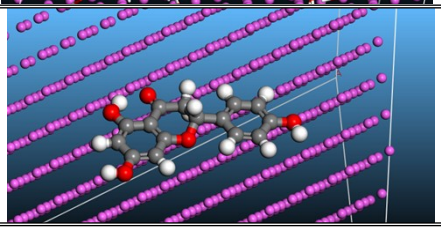
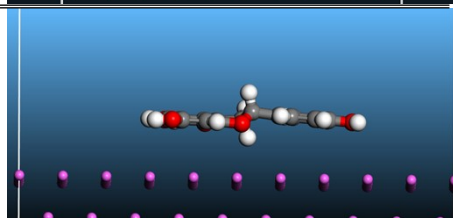
Compound		Top view	Side view
Syringic acid	protonated		
	vacuum		
Vanillic acid	neutral		
	protonated		
	vacuum		
Naringenin	neutral		
	protonated		
	vacuum		

Table B10 (continued)

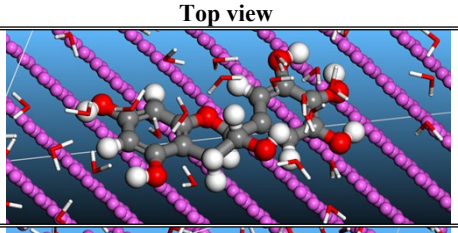
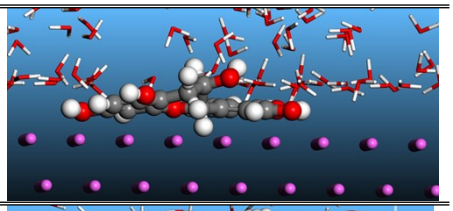
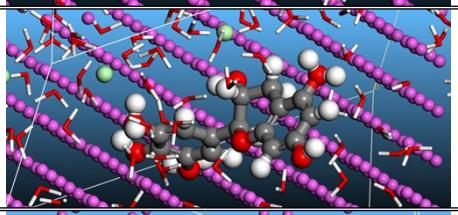
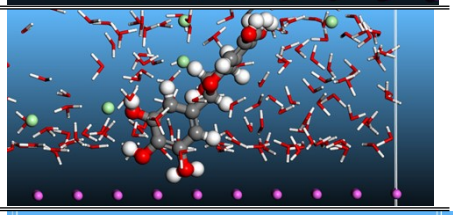
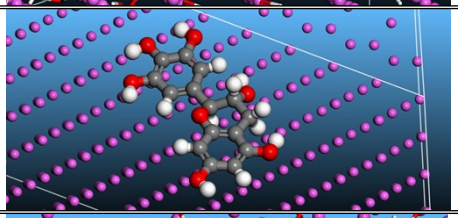
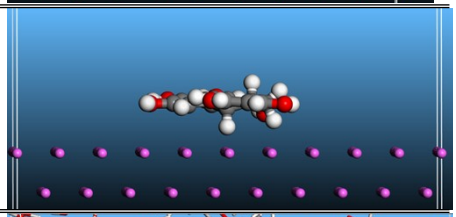
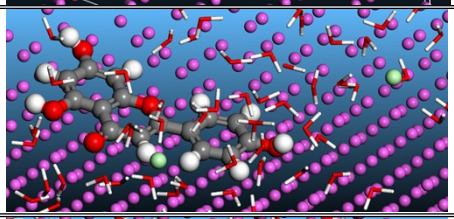
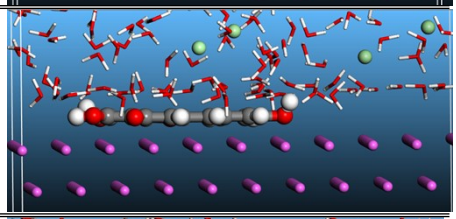
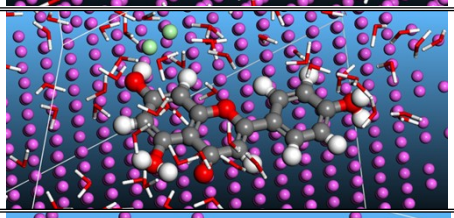
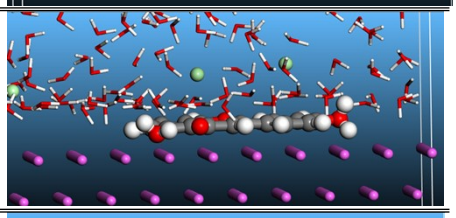
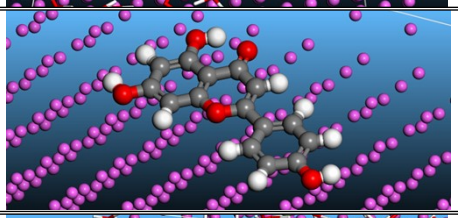
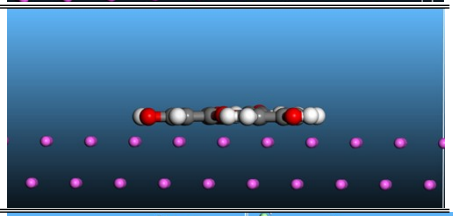
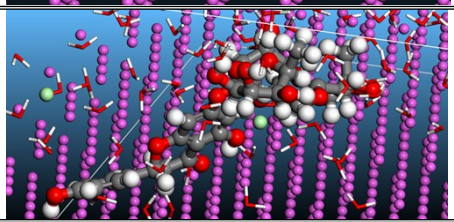
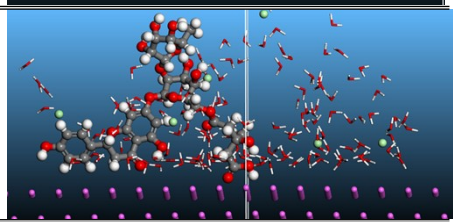
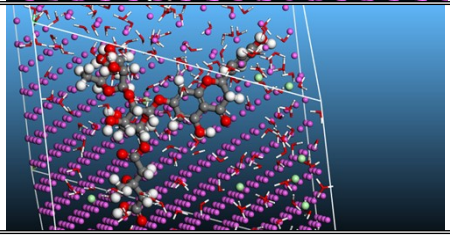
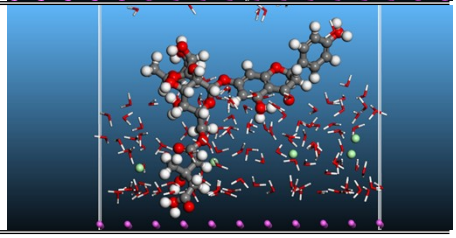
Compound		Top view	Side view
Epigallocatechin	neutral		
	protonated		
	vacuum		
Apigenin	neutral		
	protonated		
	vacuum		
Melitidin	neutral		
	protonated		

Table B10 (continued)

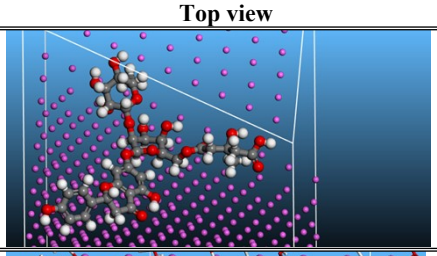
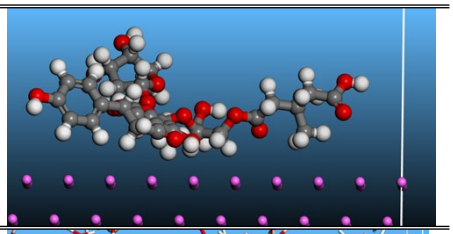
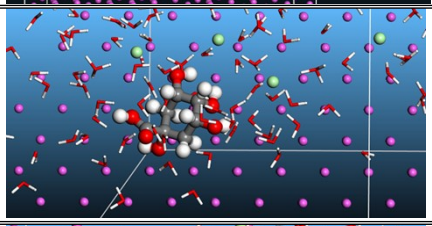
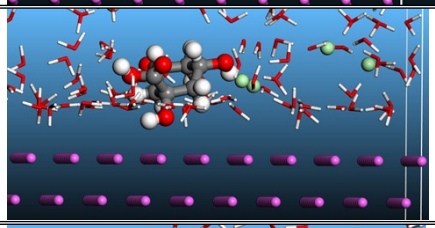
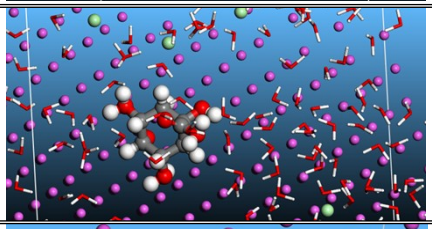
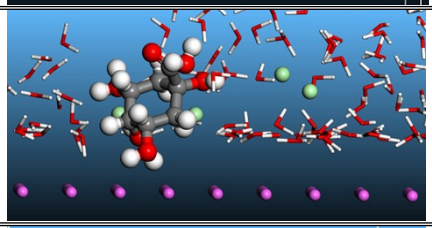
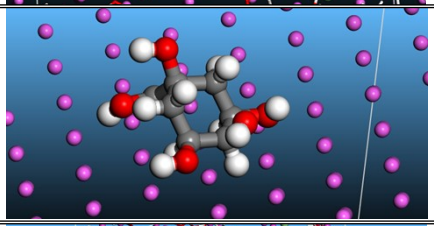
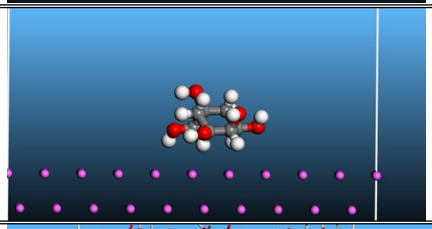
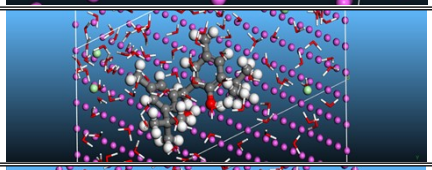
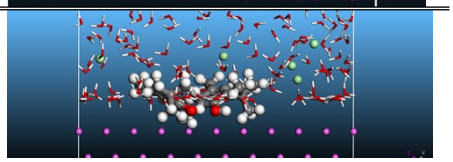
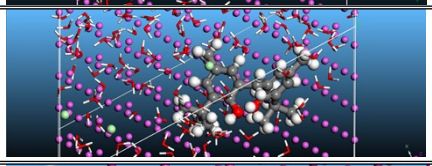
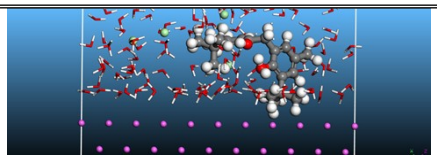
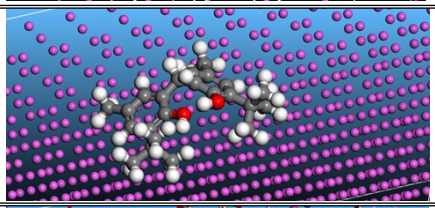
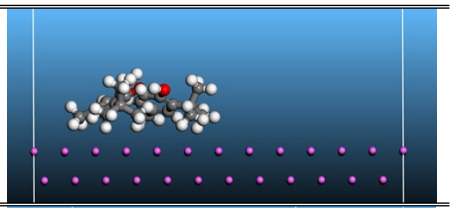
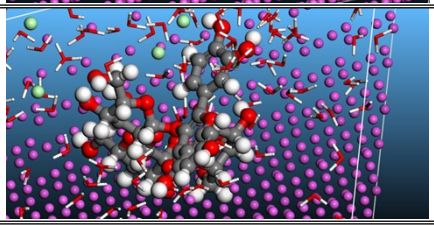
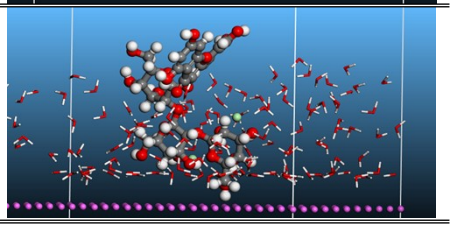
Compound		Top view	Side view
Melitidin	**vacuum**		
Quinic acid	**neutral**		
	protonated		
	vacuum		
2,2'-methylenebis	**neutral**		
	protonated		
	vacuum		
Quercetin triglucoside	**neutral**		

Table B10 (continued)

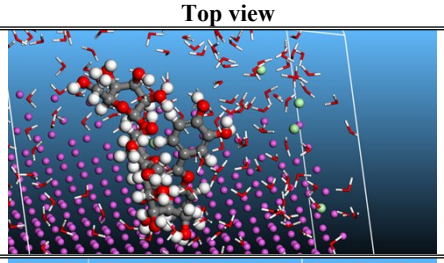
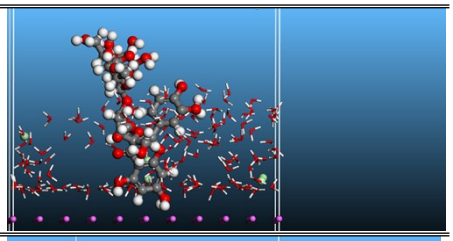
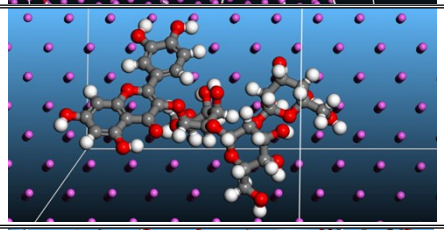
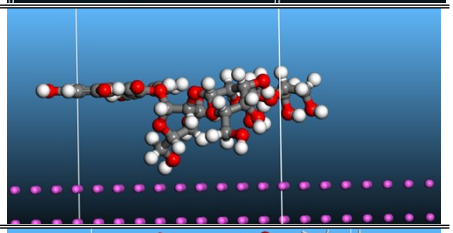
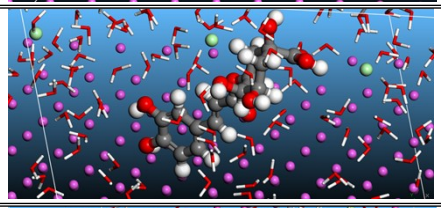
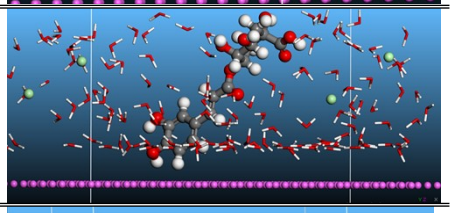
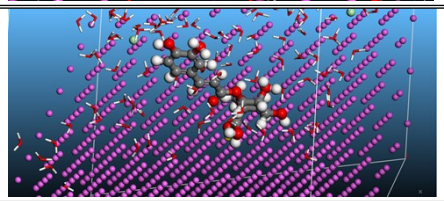
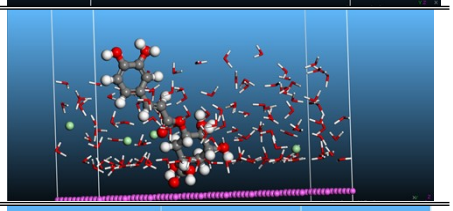
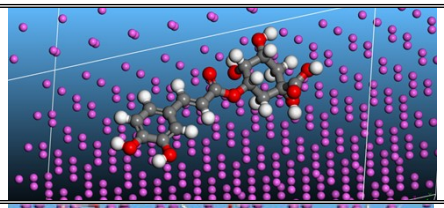
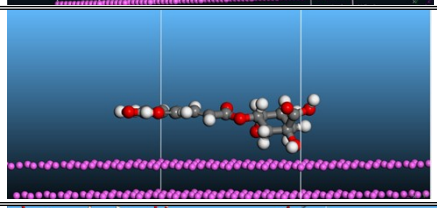
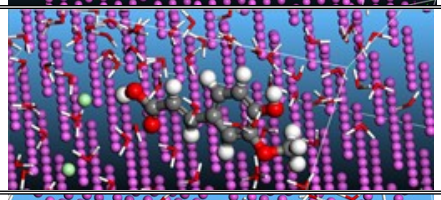
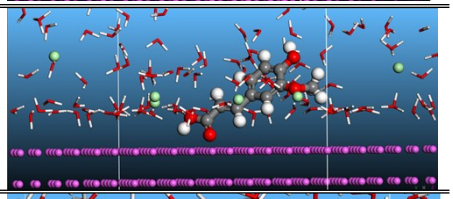
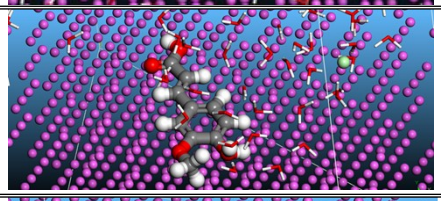
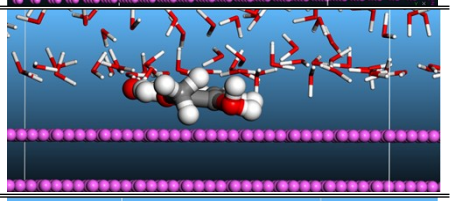
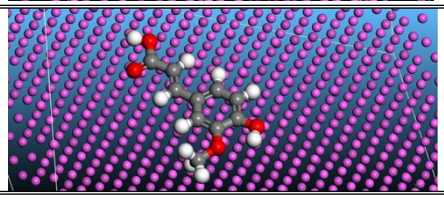
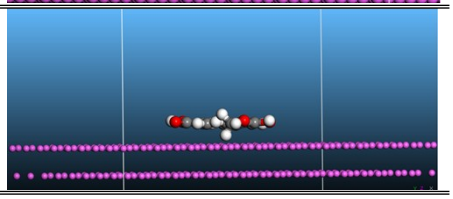
Compound		Top view	Side view
Quercetin triglucoside	protonated		
	vacuum		
Chlorogenic acid	neutral		
	protonated		
	vacuum		
Ferulic acid	neutral		
	protonated		
	vacuum		

Table B10 (continued)

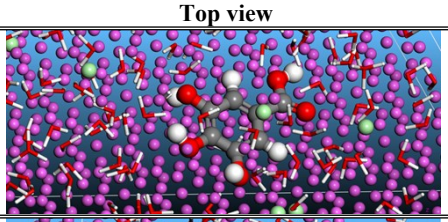
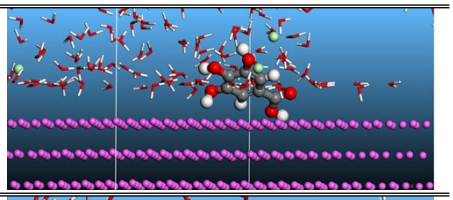
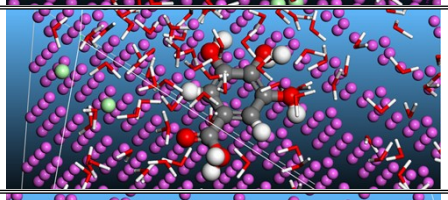
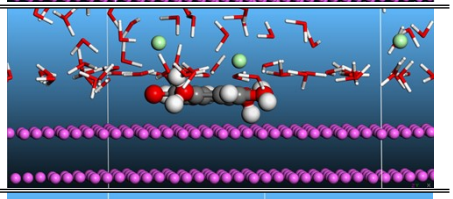
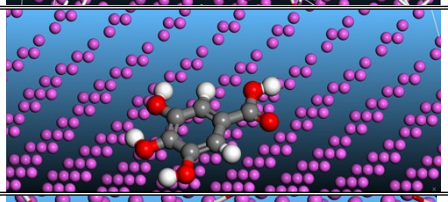
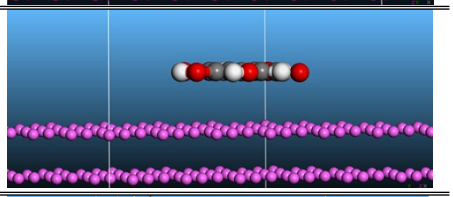
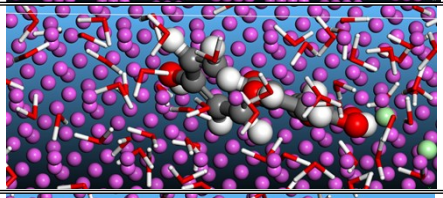
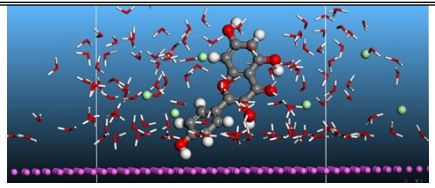
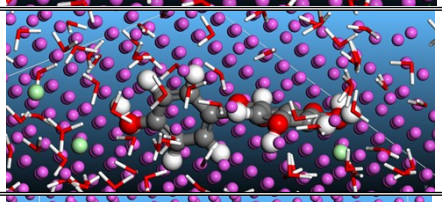
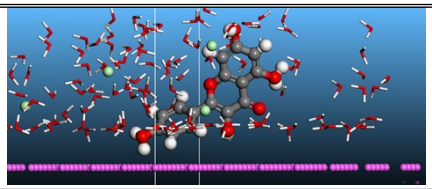
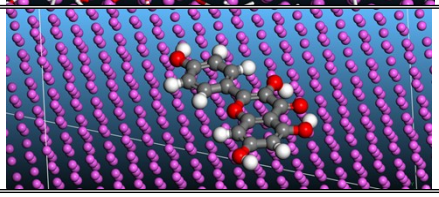
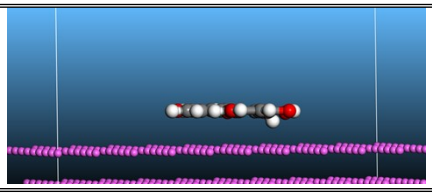
Compound		Top view	Side view
Gallic acid	neutral		
	protonated		
	vacuum		
Kaempferol	neutral		
	protonated		
	vacuum		

Table B11: Data and specifications are obtained by simulating Monte Carlo to adsorb aluminum-SCS and GPP (protonated)

Plant	Compound	Total energy (Kcal/mol)	Adsorption energy (Kcal/mol)	Rigid adsorption energy (Kcal/mol)	Deformation energy (Kcal/mol)	Hydronium ion dE_{ad}/dNi (Kcal/mol)	Water dE_{ad}/dNi (Kcal/mol)	Chloride ion dE_{ad}/dNi (Kcal/mol)	dE_{ad}/dNi (Kcal/mol)
SCS&GPP	**(+)Catechin**	-4.41E+03	-4.37E+03	-4.54E+03	161.444	-148.628	-7.754	-156.059	-53.772
SCS	**Myricetin**	-4.48E+03	-4.46E+03	-4.62E+03	167.726	-150.588	-10.602	-125.729	-68.941
SCS&GPP	**Quercetin**	-4.41E+03	-4.36E+03	-4.52E+03	159.213	-144.414	-8.134	-149.825	-63.555
SCS&GPP	**Kaempferol**	-4.47E+03	-4.42E+03	-4.58E+03	161.833	-146.613	-8.286	-138.304	-87.834
SCS	**Gallic acid**	-4.43E+03	-4.39E+03	-4.55E+03	156.248	-148.282	-6.866	-146.688	-71.450
SCS&GPP	**p-OH-benzoic acid**	-4.40E+03	-4.36E+03	-4.53E+03	164.440	-139.859	-2.463	-142.596	-31.602
SCS&GPP	**Protocatechuic acid**	-4.48E+03	-4.44E+03	-4.60E+03	162.325	-148.432	-7.491	-152.022	-79.556
SCS	**Syringic acid**	-4.38E+03	-4.40E+03	-4.57E+03	172.605	-154.471	-8.001	-145.544	-74.748
SCS	**Vanillic acid**	-4.39E+03	-4.36E+03	-4.53E+03	169.013	-127.864	-6.438	-136.926	-57.221
SCS	**Chlorogenic acid**	-4.44E+03	-4.42E+03	-4.57E+03	150.178	-152.757	-8.100	-141.129	-107.842
SCS&GPP	**Caffeic acid**	-4.49E+03	-4.38E+03	-4.54E+03	167.177	-141.792	-1.560	-141.371	-39.298
SCS	**p-Coumaric acid**	-4.48E+03	-4.38E+03	-4.55E+03	165.751	-141.617	-7.865	-131.290	-84.917
SCS	**Ferulic acid**	-4.47E+03	-4.41E+03	-4.57E+03	165.193	-148.964	-8.614	-134.713	-89.986
GPP	**Naringenin**	-4.53E+03	-4.47E+03	-4.63E+03	164.612	-142.478	-2.707	-131.342	-115.531
GPP	**Epigallocatechin**	-4.44E+03	-4.41E+03	-4.58E+03	165.107	-149.128	-7.765	-133.438	-79.092
GPP	**Apigenin**	-4.49E+03	-4.41E+03	-4.56E+03	152.904	-152.410	-2.926	-140.279	-118.466
GPP	**Melitidin**	-4.44E+03	-4.49E+03	-4.56E+03	63.930	-152.106	-6.706	-140.323	-232.402
GPP	**Quinic acid**	-4.39E+03	-4.39E+03	-4.56E+03	166.578	-149.432	-7.908	-145.082	-41.652
GPP	**2,2'-methylenebis**	-4.46E+03	-4.41E+03	-4.58E+03	169.055	-149.897	-6.702	-149.571	-80.030
GPP	**Quercetin triglucoside**	-4.31E+03	-4.57E+03	-4.65E+03	78.858	-155.896	-9.162	-141.541	-302.041

Table B12: Data and specifications are obtained by simulating Monte Carlo to adsorb aluminum-SCS and GPP (vacuum form)

Plant	Compound	Total energy (Kcal/mol)	Adsorption energy (Kcal/mol)	Rigid adsorption energy (Kcal/mol)	Deformation energy (Kcal/mol)	dE_{ad}/dNi (Kcal/mol)
SCS&GPP	**(+)Catechin**	-96.580	-67.840	-69.407	1.567	-67.840
SCS	**Myricetin**	-130.304	-90.890	-78.899	-11.992	-90.890
SCS&GPP	**Quercetin**	-125.072	-83.756	-76.424	-7.332	-83.756
SCS&GPP	**Kaempferol**	-124.335	-81.791	-74.334	-7.457	-81.791
SCS	**Gallic acid**	-66.800	-42.398	-42.485	0.087	-42.398
SCS&GPP	**p-OH-benzoic acid**	-62.933	-37.680	-37.767	0.086	-37.680
SCS&GPP	**Protocatechuic acid**	-62.913	-40.049	-40.142	0.093	-40.049
SCS	**Syringic acid**	-45.287	-53.676	-54.194	0.518	-53.676
SCS	**Vanillic acid**	-54.365	-45.847	-46.120	0.273	-45.847
SCS	**Chlorogenic acid**	-104.121	-81.983	-79.904	-2.079	-81.983
SCS&GPP	**Caffeic acid**	-131.878	-48.509	-48.587	0.078	-48.509
SCS	**p-Coumaric acid**	-131.378	-46.245	-46.332	0.087	-46.245
SCS	**Ferulic acid**	-122.732	-57.900	-54.015	-3.886	-57.900
GPP	**Naringenin**	-123.711	-79.894	-71.708	-8.186	-79.894
GPP	**Epigallocatechin**	-101.901	-75.389	-73.923	-1.466	-75.389
GPP	**Apigenin**	-154.629	-81.655	-72.208	-9.447	-81.655
GPP	**Melitidin**	-125.997	-105.297	-96.493	-8.805	-105.297
GPP	**Quinic acid**	-15.235	-37.343	-37.045	-0.298	-37.343
GPP	**2,2'-methylenebis**	-114.379	-66.674	-68.254	1.580	-66.674
GPP	**Quercetin triglucoside**	-85.350	-181.722	-140.214	-41.508	-181.722

Table B13: Analysis of variance and model summary for corrosion inhibition efficiency using GPP extract

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	287.15	9	31.91	9.87	0.0007	significant
A-Temperature	2.87	1	2.87	0.8886	0.03681	
B-Concentration	67.14	1	67.14	20.76	0.0010	
C-Time	14.87	1	14.87	4.60	0.0576	
AB	0.0101	1	0.0101	0.0031	0.9565	
AC	0.0089	1	0.0089	0.0027	0.9592	
BC	1.79	1	1.79	0.5530	0.4742	
A^2	116.50	1	116.50	36.02	0.0001	
B^2	4.80	1	4.80	1.48	0.2512	
C^2	4.78	1	4.78	1.48	0.2522	
Residual	32.34	10	3.23			
Lack of Fit	32.34	5	6.47			
Pure Error	0.0000	5	0.0000			
Cor Total	319.49	19				
Std. Dev. 1.80	R^2 0.8988					
Mean 79.14	Adjusted $R^2$0.8077					
C.V. % 2.27	Predicted R^2 0.4411					
	Adeq Precision 10.6133					

Table B14: The adequacy and significance of the corrosion rate model were evaluated through an analysis of its fit statistics and ANOVA for GPP extract

Source	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**p-value**	
Model	4.940E-08	9	5.489E-09	39.20	< 0.0001	significant
A-Temperature	2.895E-08	1	2.895E-08	206.74	< 0.0001	
B-Concentration	7.978E-10	1	7.978E-10	5.70	0.0382	
C-Time	7.098E-09	1	7.098E-09	50.68	< 0.0001	
AB	5.525E-10	1	5.525E-10	3.95	0.0751	
AC	7.440E-09	1	7.440E-09	53.13	< 0.0001	
BC	1.647E-10	1	1.647E-10	1.18	0.3036	
A^2	5.569E-09	1	5.569E-09	39.77	< 0.0001	
B^2	9.530E-11	1	9.530E-11	0.6806	0.4286	
C^2	4.462E-11	1	4.462E-11	0.3186	0.5849	
Residual	1.400E-09	10	1.400E-10			
Lack of Fit	1.400E-09	5	2.801E-10			
Pure Error	0.0000	5	0.0000			
Cor Total	5.080E-08	19				
Std. Dev. 0.0000	R^2 0.9724					
Mean 0.0000	Adjusted R^2 0.9476					
C.V. % 26.39	Predicted R^2 0.7858					
	Adeq Precision 23.300					