Molecular docking studies of seven selected medicinal plants against non-small-cell lung cancer (NSCLC) against complex of ERK2 and catechol receptor

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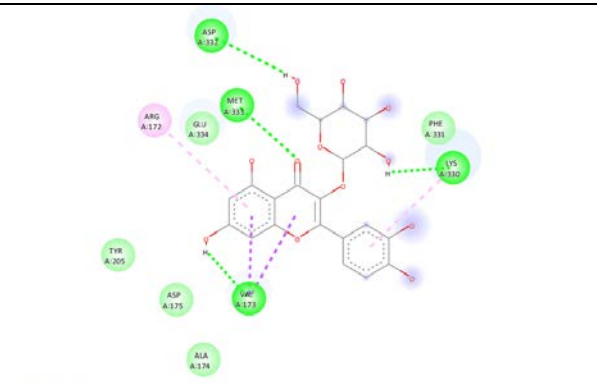
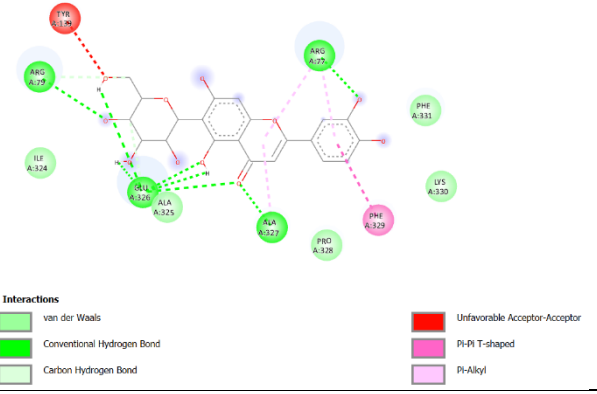
Supplementary Information

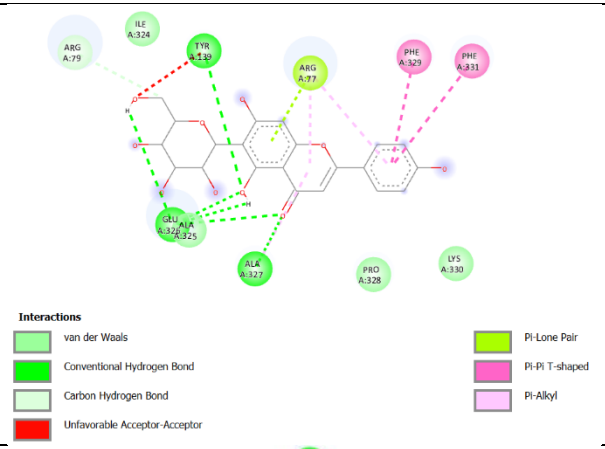
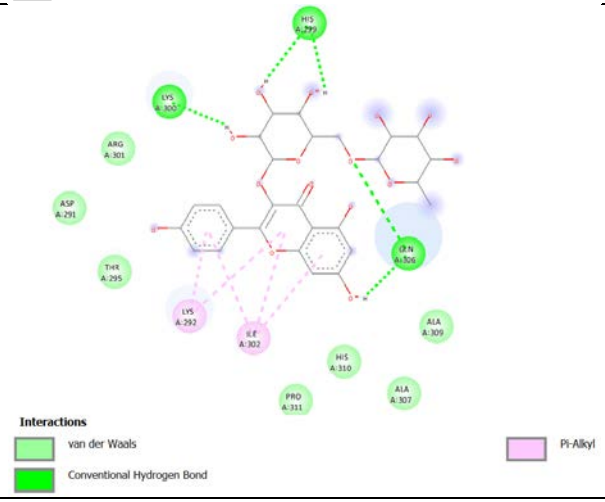
Table S1. Physicochemical properties of screened compounds from different medicinal plants

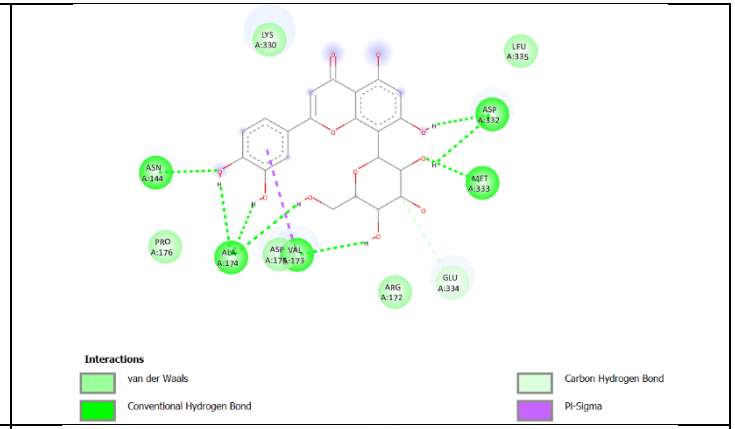
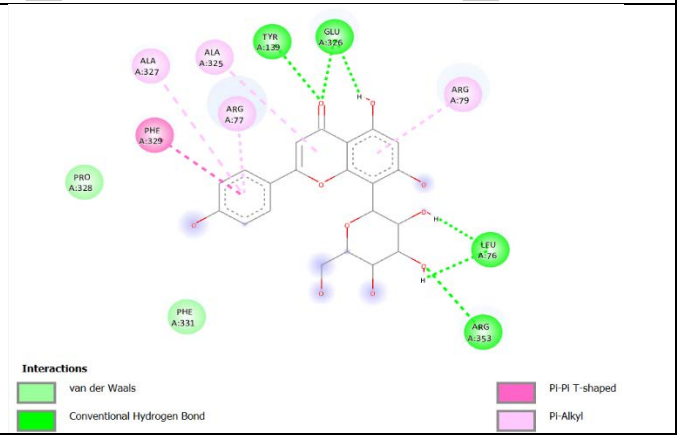
Plant Name	Compounds	PubChem Id	Molecular Weight (g/mol)	H Bond Donor	H Bond Acceptor	TPSA (Å²)	Log P (iLOGP)	Violations	Bioavailability Score
Fagopyrum esculentum	Hyperoside	5281643	464.38	8	12	210.51	2.11	2	0.17
	Isoorientin	114776	448.38	8	11	201.28	2.12	2	0.17
	Isovitexin	162350	432.38	7	10	181.05	1.94	1	0.55
	kaempferol-3-rutinoside (Nicotiflorin)	5318767	594.52	9	15	249.2	2.79	3	0.17
	Orientin	5281675	448.38	8	11	201.28	1.27	2	0.17
	Vitexin	5280441	432.38	7	10	181.05	1.38	1	0.55
Oroxylum indicum	Baicalein	5281605	270.24	3	5	90.9	2.43	0	0.55
	Baicalein-7-O-gentiobioside (Oroxin B)	10077207	594.52	9	15	249.2	1.9	3	0.17
	Baicalein-7-O-glucoside (Oroxin A)	5320313	432.38	6	10	170.05	2.54	1	0.55
	Baicalein-7-O-glucuronide (baicalin)	64982	446.36	6	11	187.12	1.59	2	0.11
	Chrysin	5281607	254.24	2	4	70.67	2.27	0	0.55
	Chrysin-7-O-beta-gentiobioside	101740041	578.52	8	14	228.97	2.81	3	0.17
	Chrysin-7-O-glucuronide	14135335	430.36	5	10	166.89	2.05	0	0.11

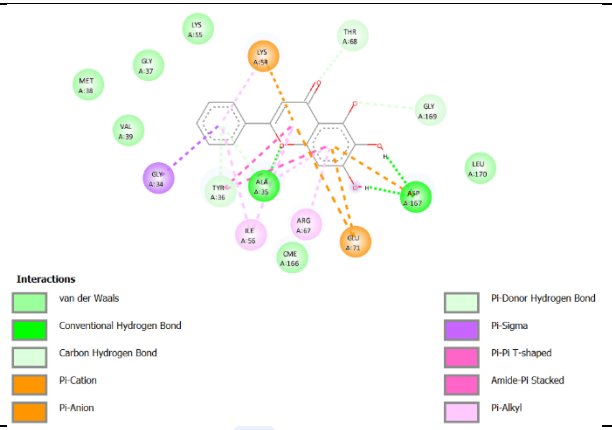
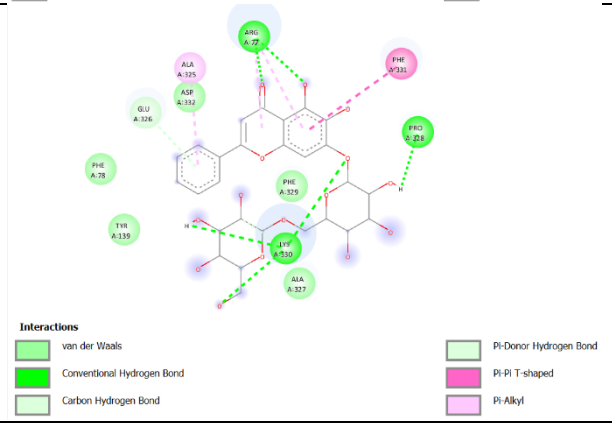
Oldenlandia diffusa	2-methyl-3-methoxy anthraquinone	10514946	252.26	0	3	43.37	2.48	0	0.55
	Quercetin 3-0-glucopyranoside	5280804	464.38	8	12	210.51	2.11	2	0.17
	Quercetin 3-0-sambubioside	5487635	596.49	10	16	269.43	1.41	3	0.17
	Quercetin 3-0-sophoroside	5282166	626.52	11	17	289.66	2.03	3	0.17
	Quercetin 3-0-rutinoside	5280805	610.52	10	16	269.43	1.28	3	0.17
Pteris multifida	Pterokaurane R	101324849	322.48	3	3	60.69	3.02	0	0.55
	2-hydroxypterosin C	21670045	250.29	3	4	77.76	1.87	0	0.55
	(2R,3S)-pterosin C	46850077	234.29	2	3	57.53	2.03	0	0.55
	(2R)-pterosin B	5320780	218.29	1	2	37.30	2.38	0	0.55
	Creticoside A	12304125	466.61	5	7	119.61	3.45	0	0.55
	Pterokaurane P1	132488069	320.47	3	3	60.69	2.86	0	0.55
Panax ginseng	Ginsenoside Rh4	21599928	620.86	6	8	139.84	4.04	2	0.17
	Ginsenoside Rh1	12855920	638.87	7	9	160.07	4.17	2	0.17
	Ginsenoside Rh5	10699455	652.90	6	9	149.07	4.57	2	0.17
	Ginsenoside Rh7	101096472	636.86	7	9	160.07	3.97	2	0.17
	Ginsenoside Rk2	90472238	604.86	5	7	119.61	5.41	1	0.55
	Ginsenoside Rk3	75412555	620.86	6	8	139.84	4.58	2	0.17
	Ginsenoside F1	9809542	638.87	7	9	160.07	3.91	2	0.17
Scrophularia nodosa	Diosmin	5281613	608.54	8	15	238.20	3.05	3	0.17
	Jionoside D	9895632	638.61	8	15	234.29	4.01	3	0.17
	Verbascoside A	15736674	668.64	7	16	235.82	4.29	3	0.17
	Verbascoside	5281800	624.59	9	15	245.29	3.00	3	0.17
Vernonia amygdalina	1,5-O-dicaffeoylquinic acid	122685	516.45	7	12	211.28	1.11	3	0.11
	3,4-O-dicaffeoylquinic acid	5281780	516.45	7	12	211.28	1.25	3	0.11
	3,5-O-dicaffeoylquinic acid	6474310	516.45	7	12	211.28	1.05	3	0.11
	4,5-Dicaffeoylquinic acid	6474309	516.45	7	12	211.28	1.25	3	0.11
	5-O-caffeoylquinic acid	5280633	354.31	6	9	164.75	0.96	1	0.11
	Glucuronolactone	92283	176.12	3	6	104.06	0.06	0	0.55

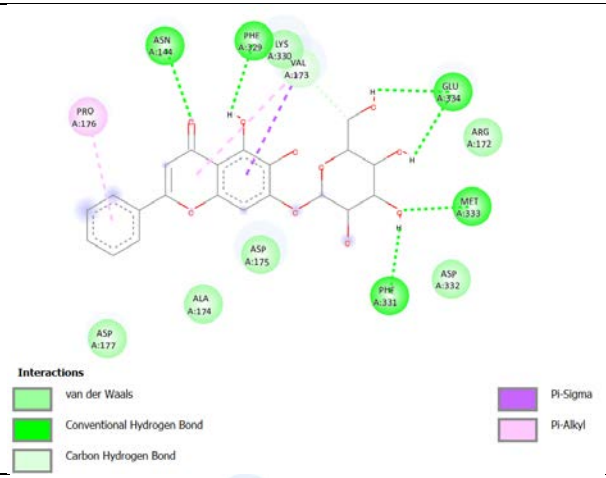
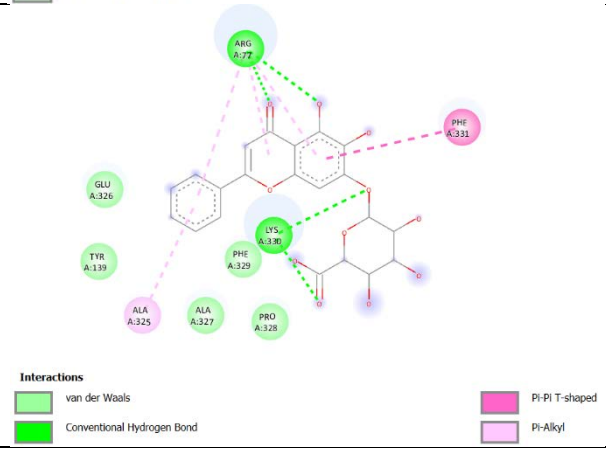
Table S2: 2D Ligand interactions generated by compounds from selected medicinal plants with Complex of ERK2 with catechol (PDB: 4ZXT) at the catalytically active site

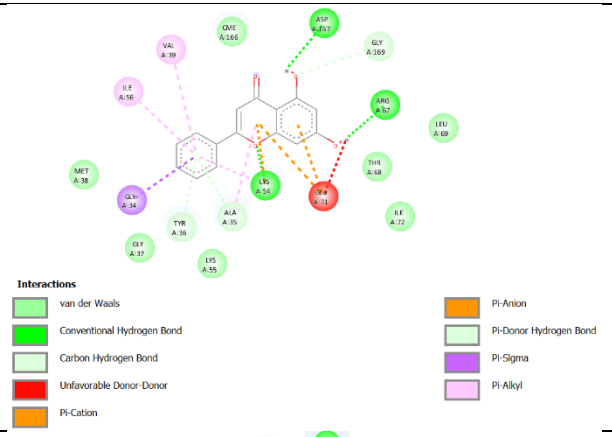
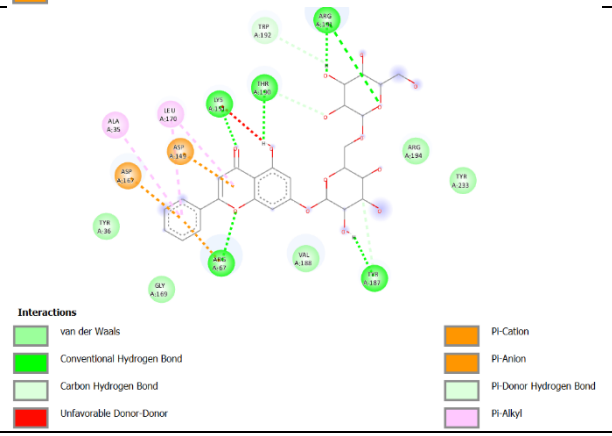
Plant Name	Compounds	Interaction
Fagopyrum esculentum	Hyperoside	
	Isoorientin	

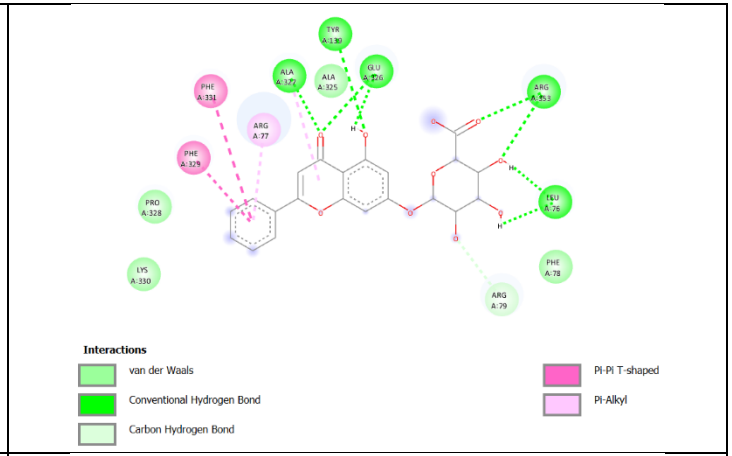
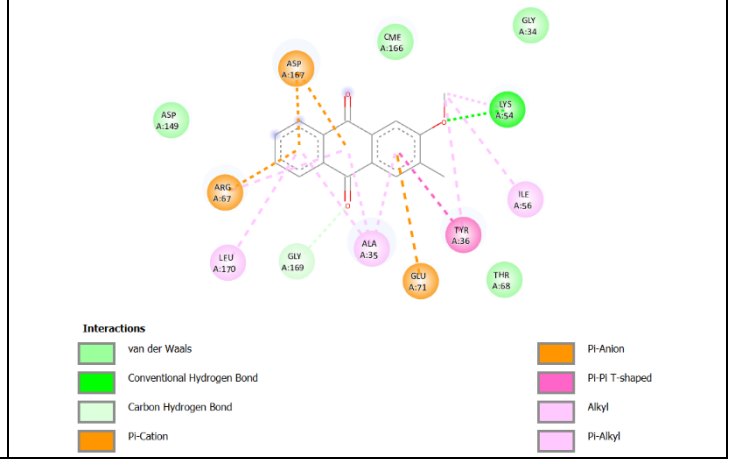
	Isovitexin	
	kaempferol-3-rutinoside (Nicotiflorin)	

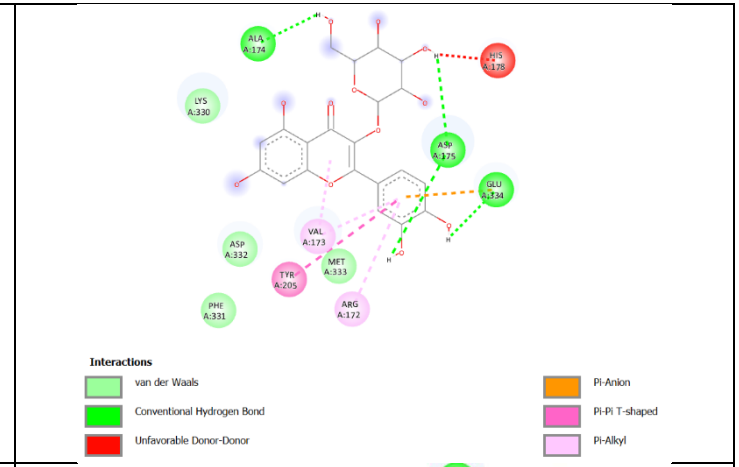
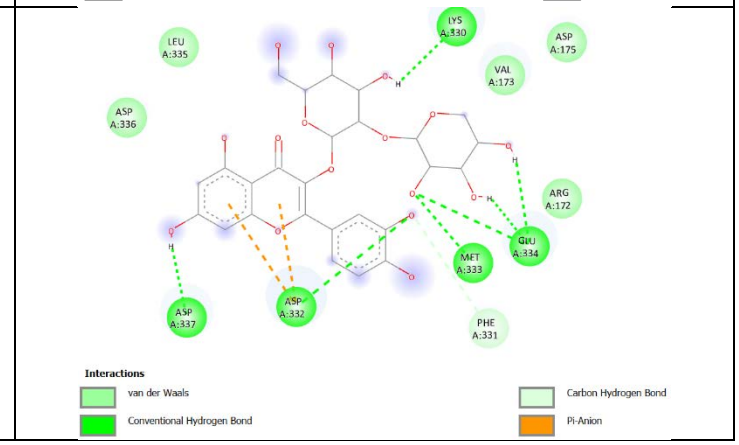
	Orientin	
	Vitexin	

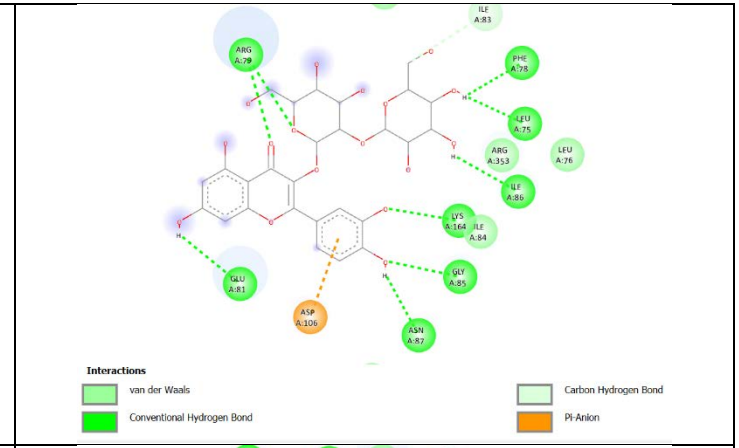
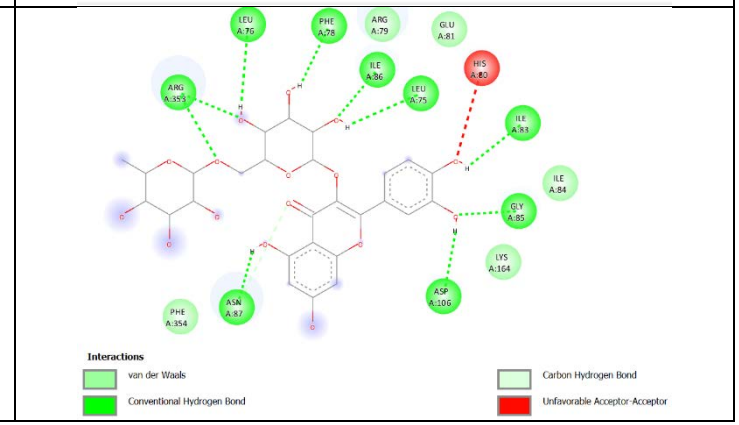
Oroxylum indicum	Baicalein	
	Baicalein-7-O-gentiobioside (Oroxin B)	

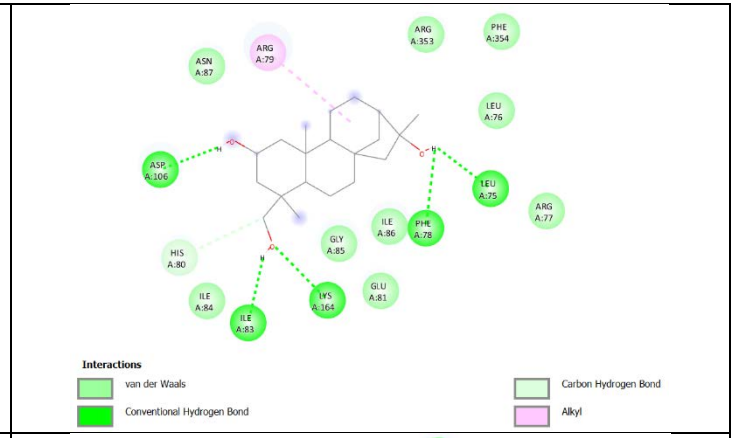
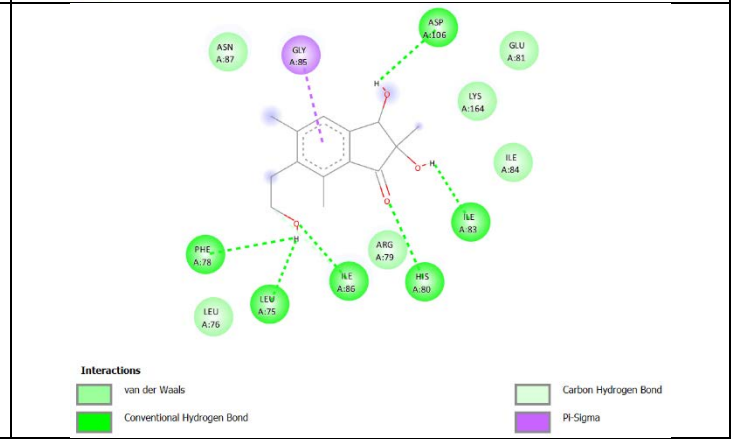
	Baicalein-7-O-glucoside (Oroxin A)	
	Baicalein-7-O-glucuronide (baicalin)	

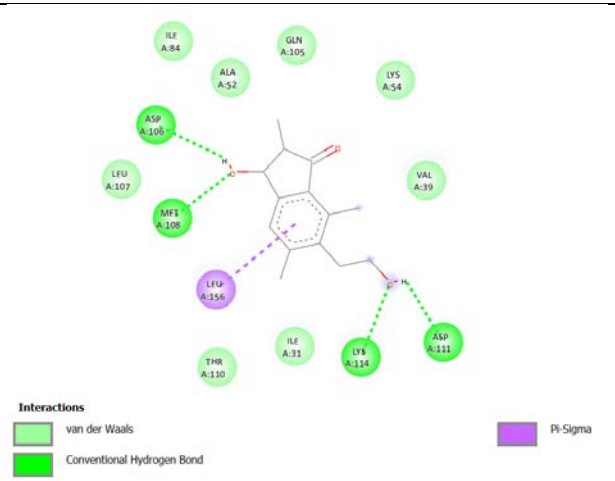
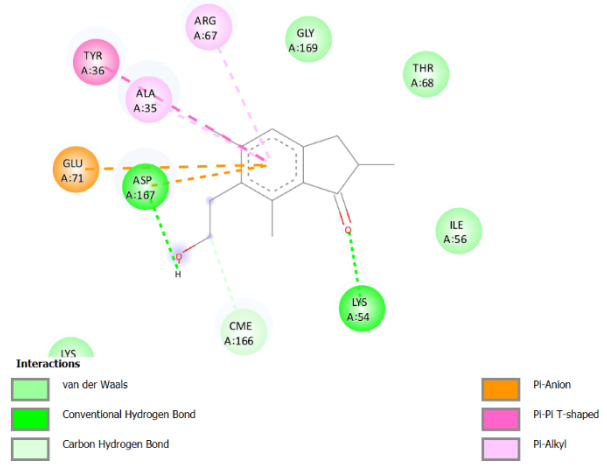
	Chrysin	
	Chrysin-7-O-beta-gentiobioside	

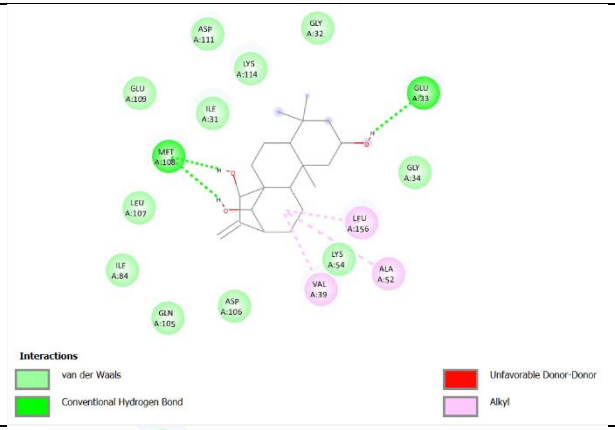
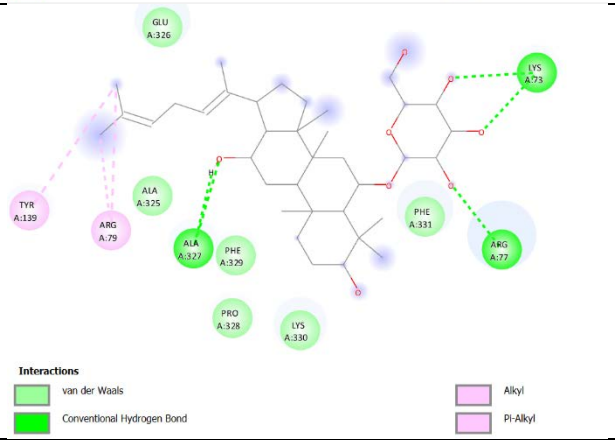
	Chrysin-7-O-glucuronide	
Oldenlandia diffusa	2-methyl-3-methoxy anthraquinone	

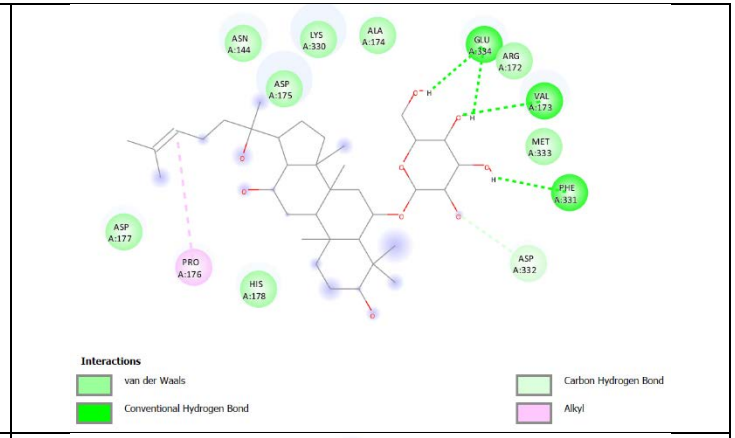
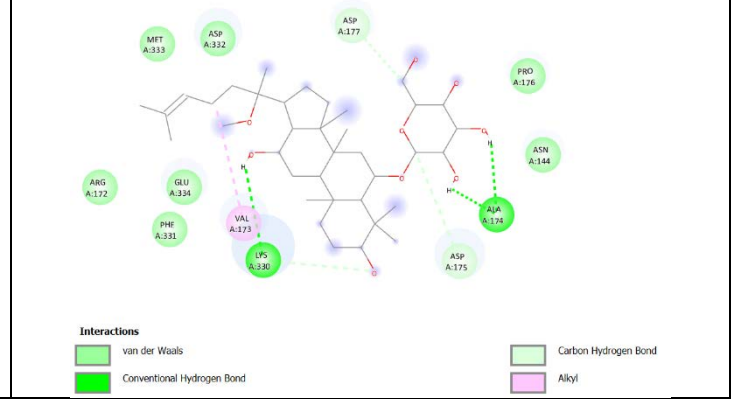
	Quercetin 3-0-glucopyranoside	
	Quercetin 3-0-sambubioside	

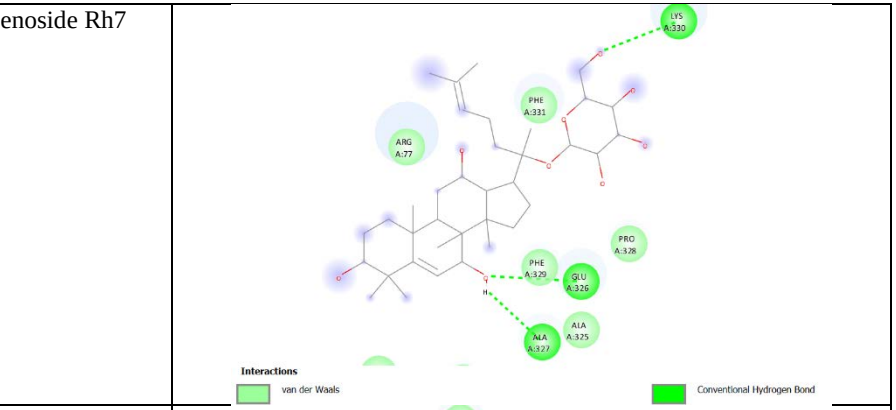
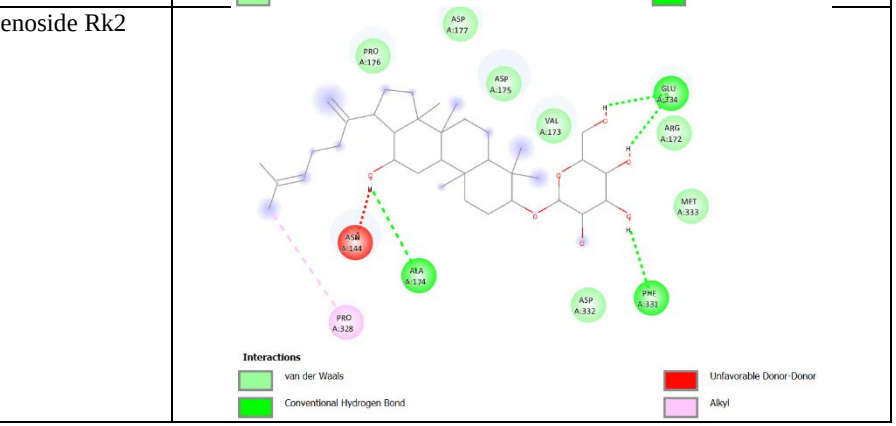
	Quercetin 3-0-sophoroside	
	Quercetin 3-0-rutinoside	

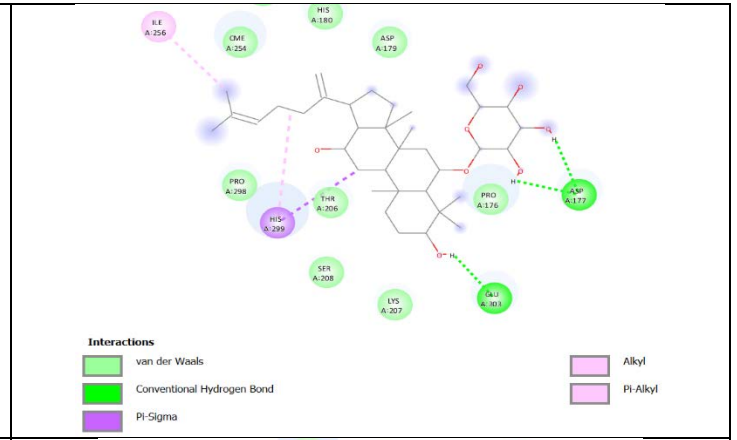
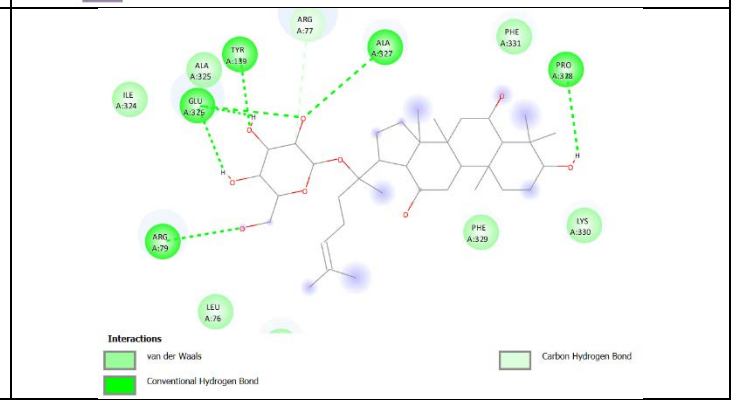
Pteris multifida	Pterokaurane R	
	2-hydroxypterosin C	

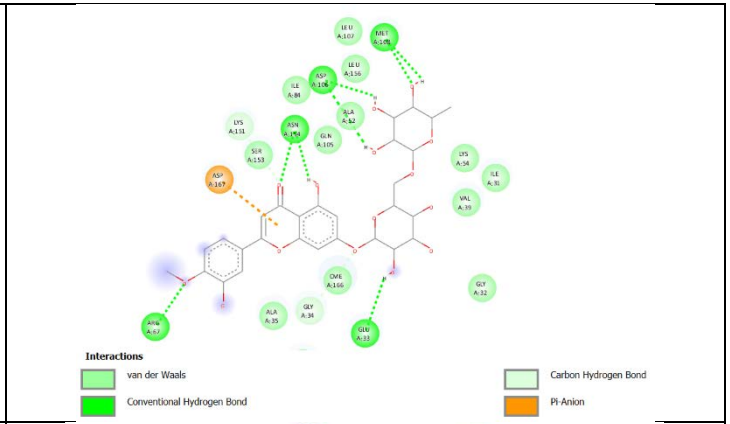
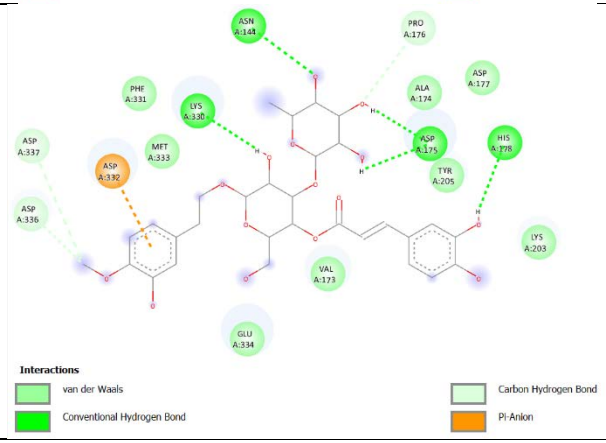
	(2R,3S)-pterosin C	
	(2R)-pterosin B	
	Creticoside A	

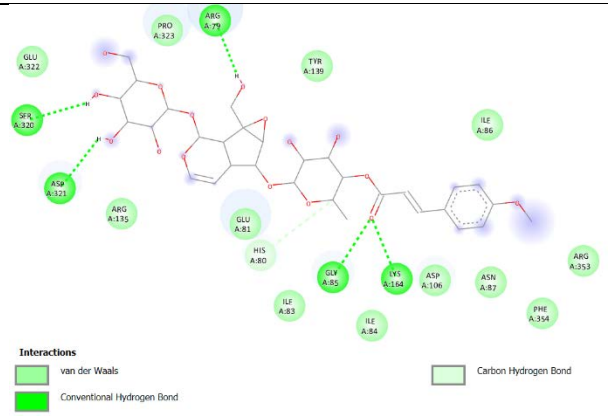
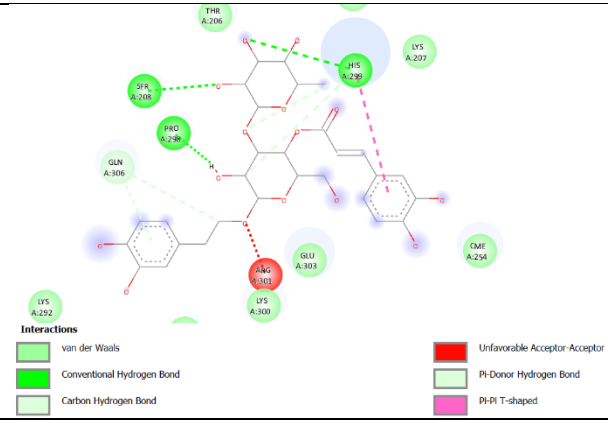
	Pterokaurane P1	
Panax ginseng	Ginsenoside Rh4	

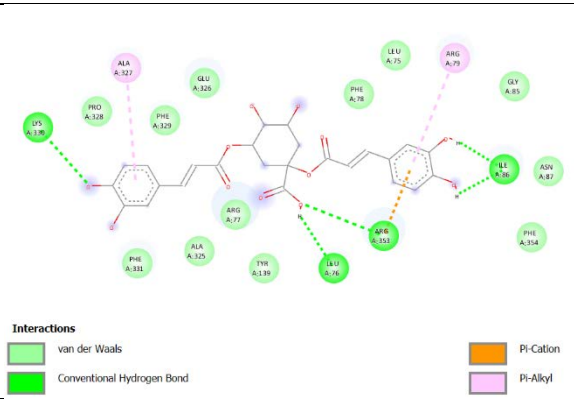
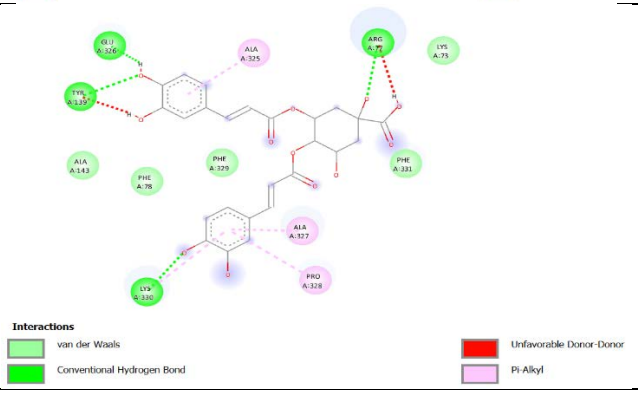
	Ginsenoside Rh1	
	Ginsenoside Rh5	

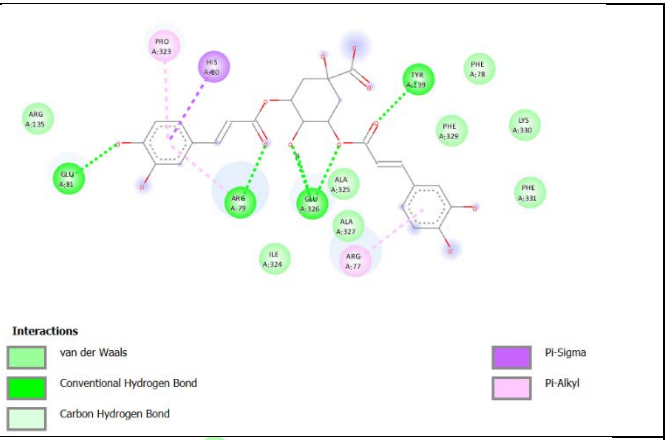
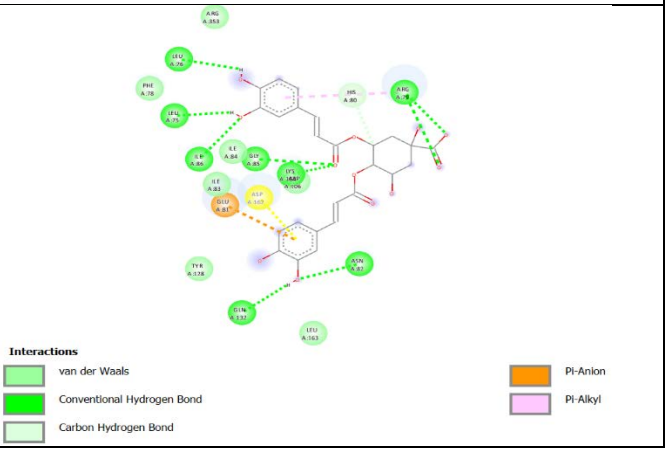
	Ginsenoside Rh7	
	Ginsenoside Rk2	

	Ginsenoside Rk3	
	Ginsenoside F1	

Scrophularia nodosa	Diosmin	
	Jionoside D	

	Verbascoside A	
	Verbascoside	

Vernonia amygdalina	1,5-O-dicaffeoylquinic acid	
	3,4-O-dicaffeoylquinic acid	

	3,5-O-dicaffeoylquinic acid = Isochlorogenic acid A	
	4,5-Dicaffeoylquinic acid	

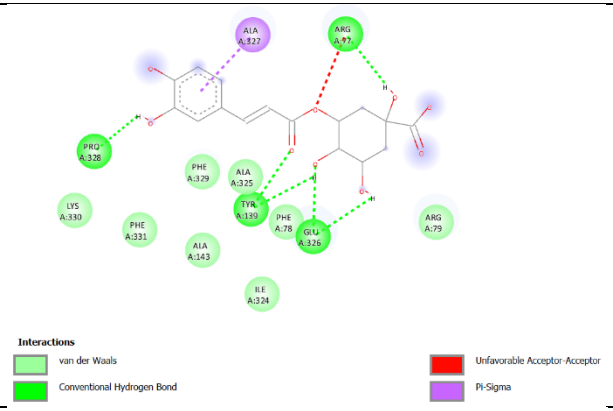
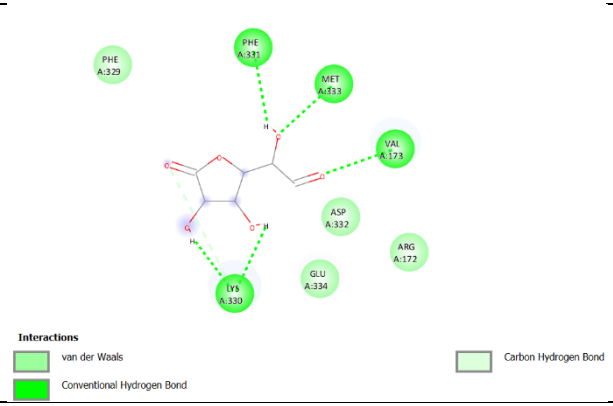
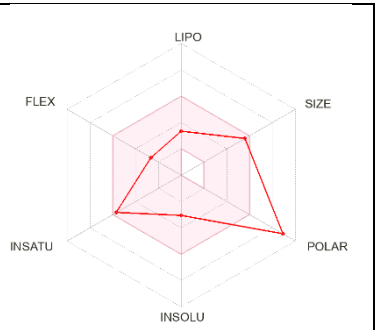
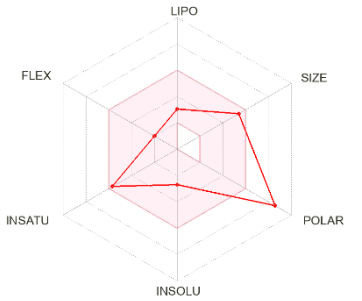
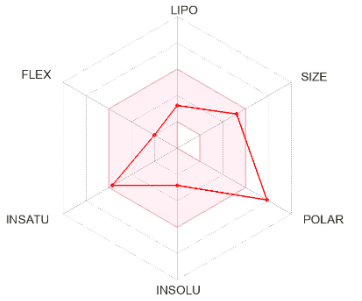
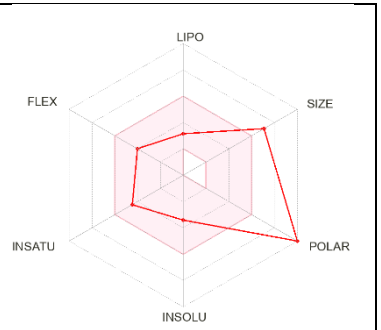
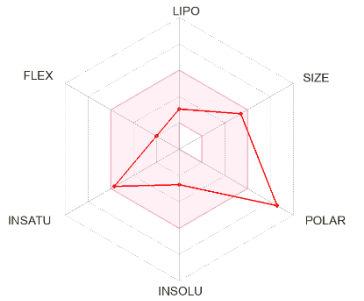
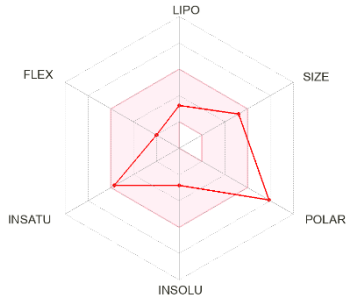
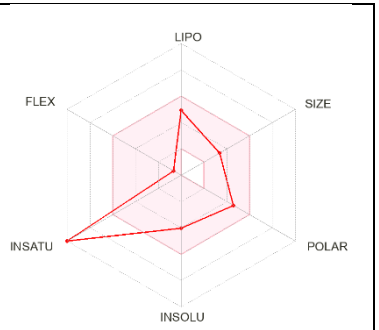
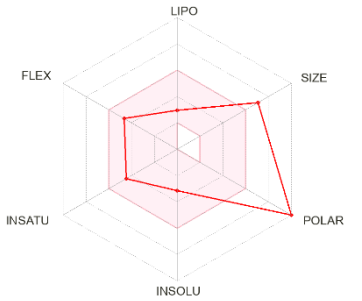
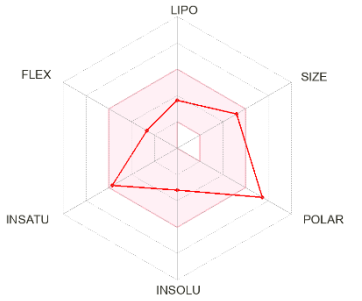
	5-O-caffeoylquinic acid = Neochlorogenic acid	
	Glucuronolactone	

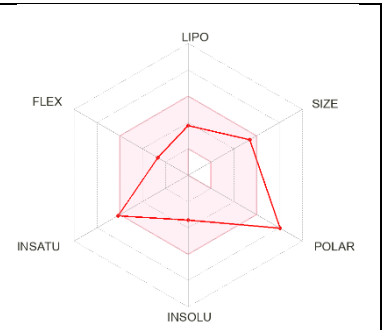
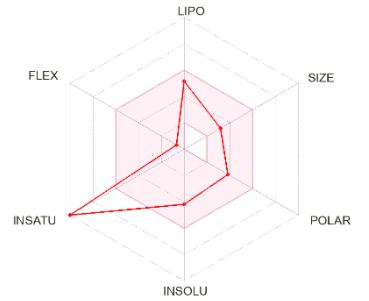
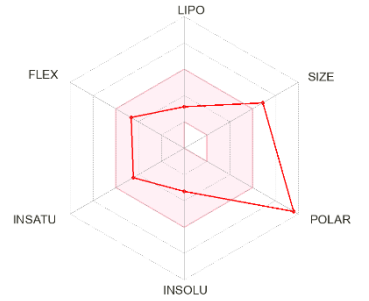
Table S3. Bioavailability Radar analysis of compounds from different medicinal plants using SwissADME

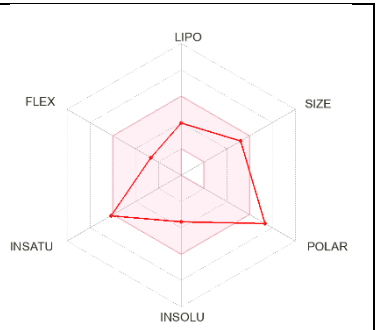
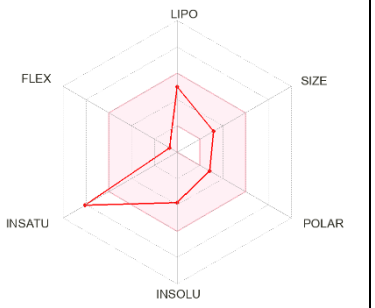
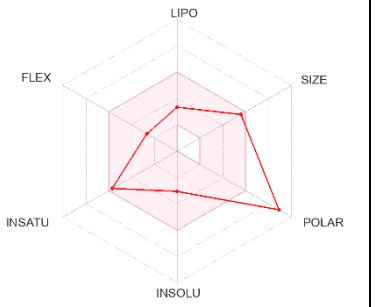
Plant Name	Compounds	Bioavailability Radar

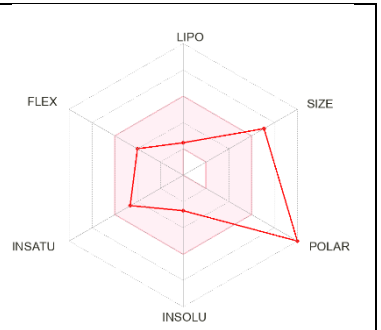
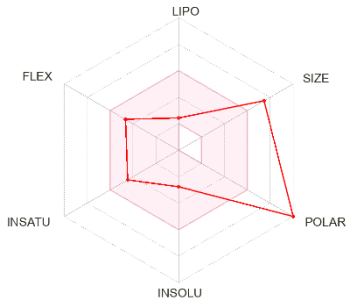
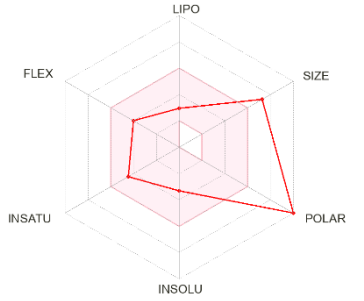
Fagopyrum esculentum	Hyperoside	
	Isoorientin	
	Isovitexin	

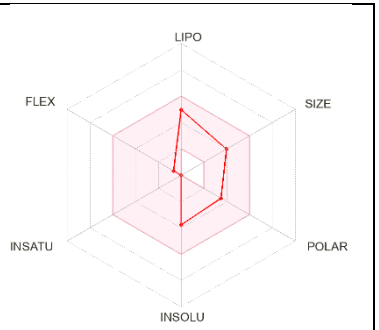
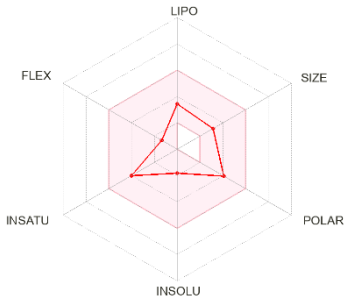
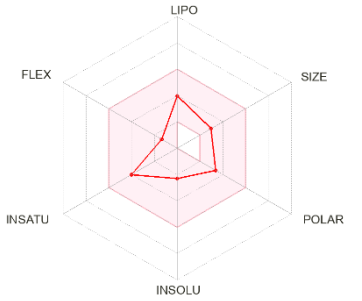
	kaempferol-3-rutinoside (Nicotiflorin)	
	Orientin	
	Vitexin	

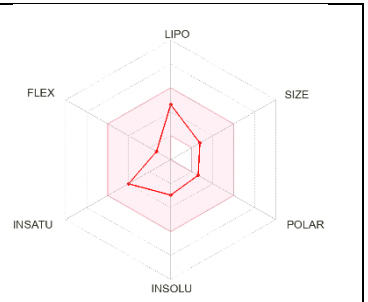
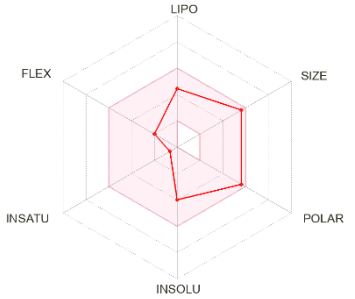
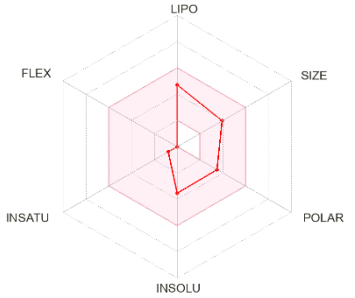
Oroxylum indicum	Baicalein	
	Baicalein-7-O-gentiobioside (Oroxin B)	
	Baicalein-7-O-glucoside (Oroxin A)	

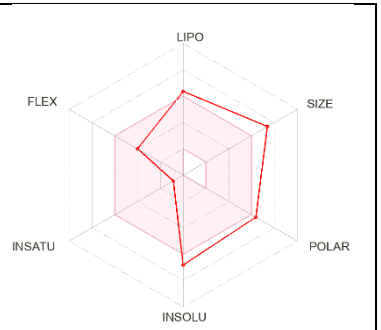
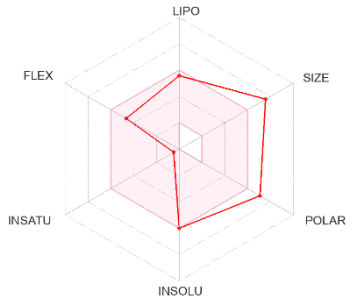
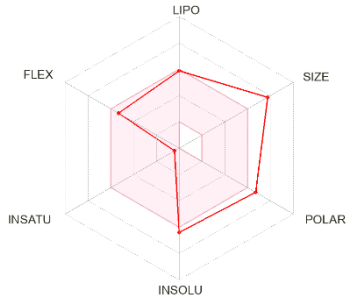
	Baicalein-7-O-glucuronide (baicalin)	
	Chrysin	
	Chrysin-7-O-beta-gentiobioside	

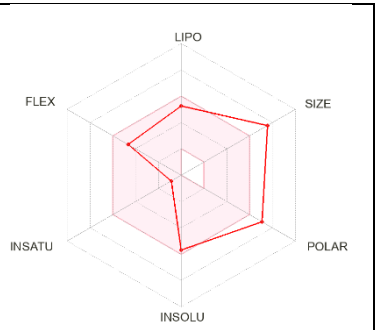
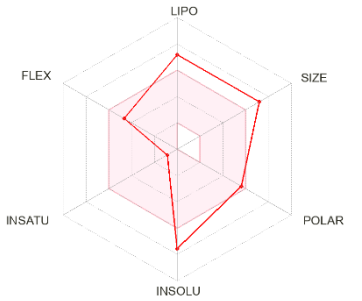
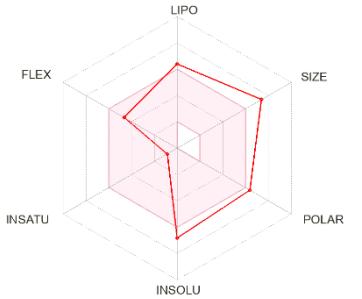
	Chrysin-7-O-glucuronide	
Oldenlandia diffusa	2-methyl-3-methoxy anthraquinone	
	Quercetin 3-0-glucopyranoside	

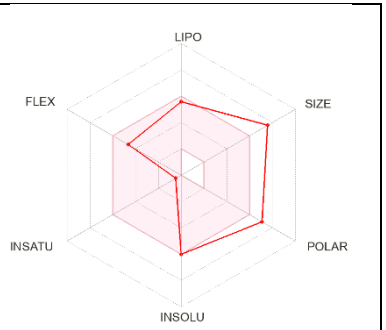
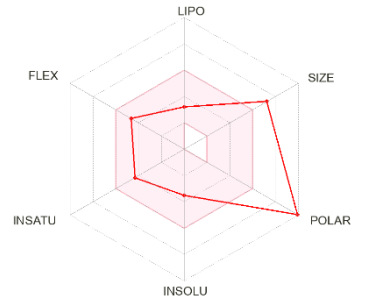
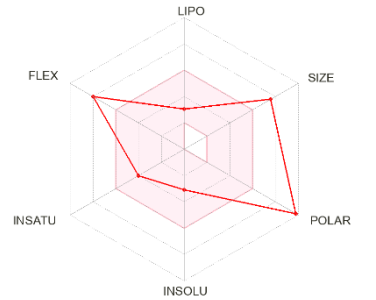
	Quercetin 3-0-sambubioside	
	Quercetin 3-0-sophoroside	
	Quercetin 3-0-rutinoside	

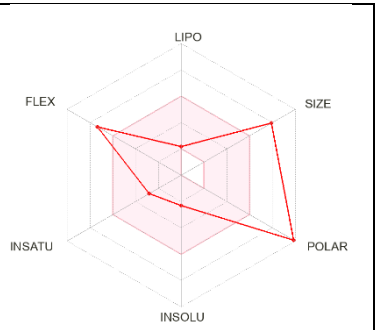
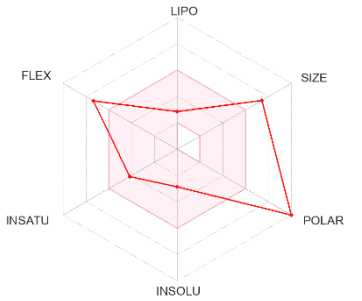
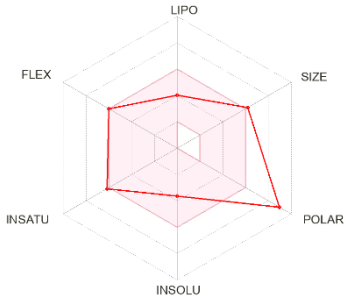
Pteris multifida	Pterokaurane R	
	2-hydroxypterosin C = (2S,3R)-2,3-dihydroxy-6-(2-hydroxyethyl)-2,5,7-trimethyl-3H-inden-1-one	
	(2R,3S)-pterosin C	

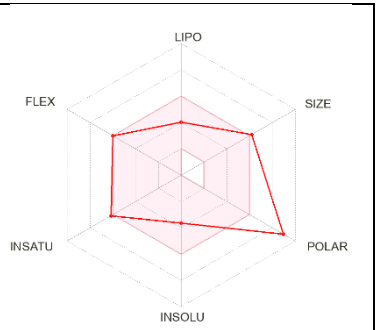
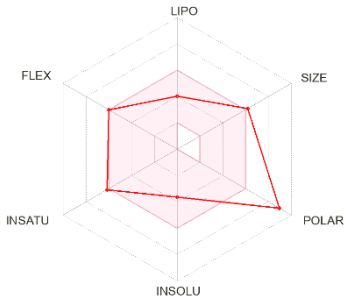
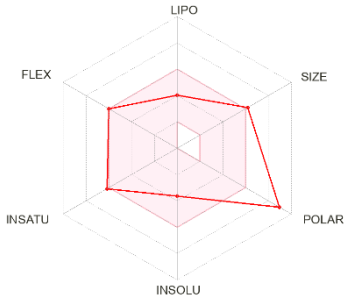
	(2R)-pterosin B	
	Creticoside A	
	Pterokaurane P1	

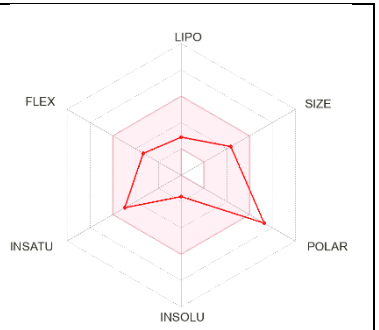
Panax ginseng	Ginsenoside Rh4	
	Ginsenoside Rh1	
	Ginsenoside Rh5	

	Ginsenoside Rh7	
	Ginsenoside Rk2	
	Ginsenoside Rk3	
	Ginsenoside F1	

		
Scrophularia nodosa	Diosmin	
	Jionoside D	

	Verbascoside A	
	Verbascoside	
Vernonia amygdalina	1,5-O-dicaffeoylquinic acid	

	3,4-O-dicaffeoylquinic acid	
	3,5-O-dicaffeoylquinic acid = Isochlorogenic acid A	
	4,5-Dicaffeoylquinic acid = Isochlorogenic acid C	

	5-O-caffeoylquinic acid = Neochlorogenic acid	
	Glucuronolactone