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**APPENDIX I****PHYTOCHEMICAL SCREENING (Harborne, 1984)**

**Detection of alkaloids:** Extracts were dissolved individually in dilute Hydrochloric acid and filtered.

- ❖ **Dragendroff's Test:** Filtrates were treated with Dragendroff's reagent (solution of Potassium Bismuth Iodide). Formation of red precipitate indicates the presence of alkaloids.
- ❖ **Hager's Test:** Filtrates were treated with Hager's reagent (saturated picric acid solution). Presence of alkaloids confirmed by the formation of yellow coloured precipitate.

**Detection of carbohydrates:** Extracts were dissolved individually in 5 ml distilled water and filtered. The filtrates were used to test for the presence of carbohydrates.

- ❖ **Molisch's Test:** Filtrates were treated with 2 drops of alcoholic  $\alpha$ -naphthol solution in a test tube. Formation of the violet ring at the junction indicates the presence of Carbohydrates.
- ❖ **Benedict's Test:** Filtrates were treated with Benedict's reagent and heated gently. Orange red precipitate indicates the presence of reducing sugars.

**Detection of glycosides:** Extracts were hydrolysed with dil. HCl, and then subjected to test for glycosides.

- ❖ **Legal's Test:** Extracts were treated with sodium nitropruside in pyridine and sodium hydroxide. Formation of pink to blood red colour indicates the presence of cardiac glycosides.

**Detection of saponins:**

- ❖ **Froth Test:** Extracts were diluted with distilled water to 20ml and this was shaken in a graduated cylinder for 15 minutes. Formation of 1 cm layer of foam indicates the presence of saponins.
- ❖ **Foam Test:** 0.5 gm of extract was shaken with 2 ml of water. If foam produced persists for ten minutes it indicates the presence of saponins.

**Detection of phytosterols:**

- ❖ **Salkowski's Test:** Extracts were treated with chloroform and filtered. The filtrates were treated with few drops of conc. sulphuric acid, shaken and allowed to stand. Appearance of golden yellow colour indicates the presence of triterpenes.
- ❖ **Liebermann Burchard's test:** Extracts were treated with chloroform and filtered. The filtrates were treated with few drops of acetic anhydride, boiled and cooled. conc. sulphuric acid was added. Formation of brown ring at the junction indicates the presence of phytosterols.

**Detection of phenols:**

- ❖ **Ferric Chloride Test:** Extracts were treated with 3-4 drops of ferric chloride solution. Formation of bluish black colour indicates the presence of phenols.

**Detection of tannins:**

- ❖ **Gelatin Test:** To the extract, 1% gelatin solution containing sodium chloride was added. Formation of white precipitate indicates the presence of tannins.

**Detection of flavonoids:**

- ❖ **Alkaline Reagent Test:** Extracts were treated with few drops of sodium hydroxide solution. Formation of intense yellow colour, which becomes colourless on addition of dilute acid, indicates the presence of flavonoids.
- ❖ **Lead acetate Test:** Extracts were treated with few drops of lead acetate solution. Formation of yellow colour precipitate indicates the presence of flavonoids.

**Detection of proteins and aminoacids:**

- ❖ **Xanthoproteic Test:** The extracts were treated with few drops of conc. Nitric acid. Formation of yellow colour indicates the presence of proteins.
- ❖ **Ninhydrin Test:** To the extract, 0.25% w/v ninhydrin reagent was added and boiled for few minutes. Formation of blue colour indicates the presence of amino acid.

**Detection of diterpenes:**

- ❖ **Copper acetate Test:** Extracts were dissolved in water and treated with 3-4 drops of copper acetate solution. Formation of emerald green colour indicates the presence of diterpenes

## APPENDIX II

## Mullikkens Charges

Compound	Atom No	Atomic No	Charge		Compound	Atom No	Atomic No	Charge	
			PM3	AM1				PM3	AM1
CAFFEIC ACID	1	8	-0.4022	-0.3627	KAEMPEROL	1	6	-0.2743	-0.2276
	2	6	-0.1534	-0.1774		2	6	0.4134	0.3349
	3	6	0.0296	0.0157		3	6	-0.3449	-0.2956
	4	6	0.0686	0.0605		4	6	0.2629	0.2188
	5	6	-0.0900	-0.1088		5	6	-0.3185	-0.2743
	6	6	-0.0831	-0.0720		6	6	0.1881	0.1685
	7	6	-0.0815	-0.0995		7	8	-0.0622	-0.0850
	8	6	0.0127	-0.0209		8	6	0.0807	0.0894
	9	6	-0.2006	-0.2025		9	6	-0.0830	-0.0690
	10	6	0.4202	0.3397		10	6	0.3933	0.3134
	11	8	-0.2393	-0.2659		11	6	0.0962	0.0896
	12	8	-0.2205	-0.2456		12	6	-0.0031	-0.0056
	20	8	-0.3099	-0.3229		13	6	-0.1869	-0.1587
	14	1	0.1259	0.1586		14	6	0.3506	0.2988
	15	1	0.1154	0.1415		15	6	-0.2657	-0.2444
	16	1	0.1154	0.1499		16	6	0.0064	0.0054
	17	1	0.1303	0.1560		17	8	-0.1963	-0.2081
	18	1	0.2108	0.2324		18	8	-0.1571	-0.1700
	19	1	0.2104	0.2381		19	8	-0.2062	-0.2200
	13	1	0.1127	0.1405		20	8	-0.2089	-0.2296
	21	1	0.2283	0.2452		21	8	-0.3749	-0.3433
				22	1	0.2278	0.2575		
				23	1	0.2282	0.2612		
				24	1	0.2179	0.2456		
				25	1	0.2167	0.2481		
APIGENIN	1	6	-0.2482	-0.2351	LUTEOLIN	1	6	-0.2492	-0.2357
	2	6	0.2028	0.1698		2	6	0.2037	0.1706
	3	6	-0.3072	-0.2981		3	6	-0.3073	-0.2978
	4	6	0.2675	0.2220		4	6	0.2682	0.2227
	5	6	-0.3680	-0.3130		5	6	-0.3685	-0.3132
	6	6	0.1885	0.1675		6	6	0.1888	0.1677
	7	8	-0.0985	-0.1350		7	8	-0.0998	-0.1366
	8	6	0.1711	0.1546		8	6	0.1655	0.1505
	9	6	-0.3040	-0.3022		9	6	-0.2992	-0.2968
	10	6	0.4131	0.3292		10	6	0.4125	0.3287
	11	6	-0.1249	-0.1086		11	6	-0.0841	-0.0723
	12	6	-0.0303	-0.0610		12	6	-0.0651	-0.0889
	13	6	-0.1493	-0.1647		13	6	-0.1248	-0.1437
	14	6	0.1230	0.1051		14	6	0.0977	0.0929
	15	6	-0.2040	-0.2230		15	6	0.0059	-0.0124
	16	6	-0.0139	-0.0439		16	6	-0.1106	-0.1271
	17	8	-0.2208	-0.2440		17	8	-0.2165	-0.2405
	18	8	-0.2217	-0.2402		18	8	-0.2217	-0.2401
	19	8	-0.2539	-0.2507		19	8	-0.2533	-0.2500
	20	8	-0.3835	-0.3512		20	8	-0.3818	-0.3490
	21	1	0.2577	0.2681		24	8	-0.2405	-0.2686

Compound	Atom No	Atomic No	Charge		Compound	Atom No	Atomic No	Charge	
			PM3	AM1				PM3	AM1
	22	1	0.2048	0.2289		22	1	0.2052	0.2294
	23	1	0.2006	0.2236		23	1	0.2126	0.2417
	24	1	0.1459	0.1724		21	1	0.2577	0.2683
	25	1	0.1375	0.1603		25	1	0.2111	0.2329
	26	1	0.1128	0.1463		26	1	0.1455	0.1715
	27	1	0.1275	0.1584		27	1	0.1379	0.1608
	28	1	0.1129	0.1520		28	1	0.1155	0.1479
	29	1	0.1462	0.1708		29	1	0.1270	0.1612
	30	1	0.1161	0.1413		30	1	0.1202	0.1538
							31	1	0.1469
TECOMOSIDE	1	6	0.0284	0.0051	QUERCETIN	1	6	-0.2395	-0.2395
	2	8	-0.0087	-0.0514		2	6	0.1789	0.1789
	3	6	-0.0159	0.0287		3	6	-0.3017	-0.3017
	4	6	-0.3979	-0.3668		4	6	0.2273	0.2273
	5	6	0.2464	0.2187		5	6	-0.3144	-0.3144
	6	6	-0.1858	-0.1851		6	6	0.17697	0.1769
	7	6	-0.0326	-0.0379		7	8	-0.1246	-0.1246
	8	6	0.0450	0.0328		8	6	0.09825	0.0982
	9	6	-0.1251	-0.1464		9	6	-0.0917	-0.0917
	10	6	0.3554	0.2515		10	6	0.30928	0.3093
	12	8	-0.3401	-0.2970		11	6	-0.0523	-0.0523
	14	8	-0.0468	-0.0732		12	6	-0.0780	-0.0780
	15	6	-0.1168	-0.1666		13	6	-0.1471	-0.1471
	16	8	-0.2158	-0.2379		14	6	0.08923	0.0892
	17	8	-0.3696	-0.4065		15	6	-0.0156	-0.0156
	11	1	0.0724	0.1139		16	6	-0.1339	-0.1339
	13	1	0.1883	0.2054		17	8	-0.2428	-0.2428
	18	1	0.1517	0.1913		18	8	-0.2374	-0.2374
	19	1	0.1994	0.2214		19	8	-0.2464	-0.2464
	20	1	0.1659	0.2125		20	8	-0.2431	-0.2432
	21	1	0.1880	0.2048		21	8	-0.3619	-0.3619
	22	1	0.1109	0.1429		26	8	-0.2706	-0.2706
	23	1	0.1034	0.1393		23	1	0.2308	0.2308
				24	1	0.2446	0.2446		
				25	1	0.2396	0.2396		
				22	1	0.26640	0.2664		
				27	1	0.23058	0.2305		
				28	1	0.17429	0.1742		
				29	1	0.16241	0.1624		
				30	1	0.16441	0.1644		
				31	1	0.15906	0.1590		
				32	1	0.14942	0.1494		

Compound	Atom No	Atomic No	Charge	
			PM3	AM1
PHYTOL	1	6	-0.0768	-0.1066
	2	6	-0.1109	-0.2085
	3	6	-0.1007	-0.1544
	4	6	-0.1210	-0.1587
	5	6	-0.0997	-0.1548
	6	6	-0.0787	-0.1062
	7	6	-0.1267	-0.2100
	8	6	-0.1150	-0.1573
	9	6	-0.1071	-0.1569
	10	6	-0.0625	-0.1298
	11	6	-0.1094	-0.0989
	12	6	-0.0713	-0.870
	13	6	-0.1851	-0.2322
	14	6	0.2662	0.1336
	16	6	-0.1204	-0.2080
	44	8	-0.3066	-0.2770
	17	1	0.0608	0.0845
	18	1	0.0402	0.0728
	19	1	0.0387	0.0711
	20	1	0.0395	0.0726
	21	1	0.0516	0.0774
	22	1	0.0536	0.0806
	23	1	0.0603	0.0835
	24	1	0.0579	0.0779
	25	1	0.0533	0.0796
	26	1	0.0534	0.0817
	27	1	0.0652	0.0857
	28	1	0.0426	0.0752
	29	1	0.0438	0.0763
	30	1	0.0470	0.0681
	31	1	0.0622	0.0832
	32	1	0.0548	0.0820
	33	1	0.0542	0.0808
	34	1	0.0561	0.0738
	35	1	0.0570	0.0902
	36	1	0.0538	0.0895
	37	1	0.0467	0.0824
	38	1	0.0473	0.0826
	39	1	0.0444	0.0800
	40	1	0.0868	0.1050
	41	1	0.0416	0.0732
	42	1	0.0404	0.0717
	43	1	0.0458	0.0747
	15	1	0.0191	0.0738
	45	1	0.0879	0.1133
	46	1	0.0190	0.0687