

Supplementary File S1: Gas Chromatographic Mass spectrometric Studies

Figure S1: Chromatogram of Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Roots

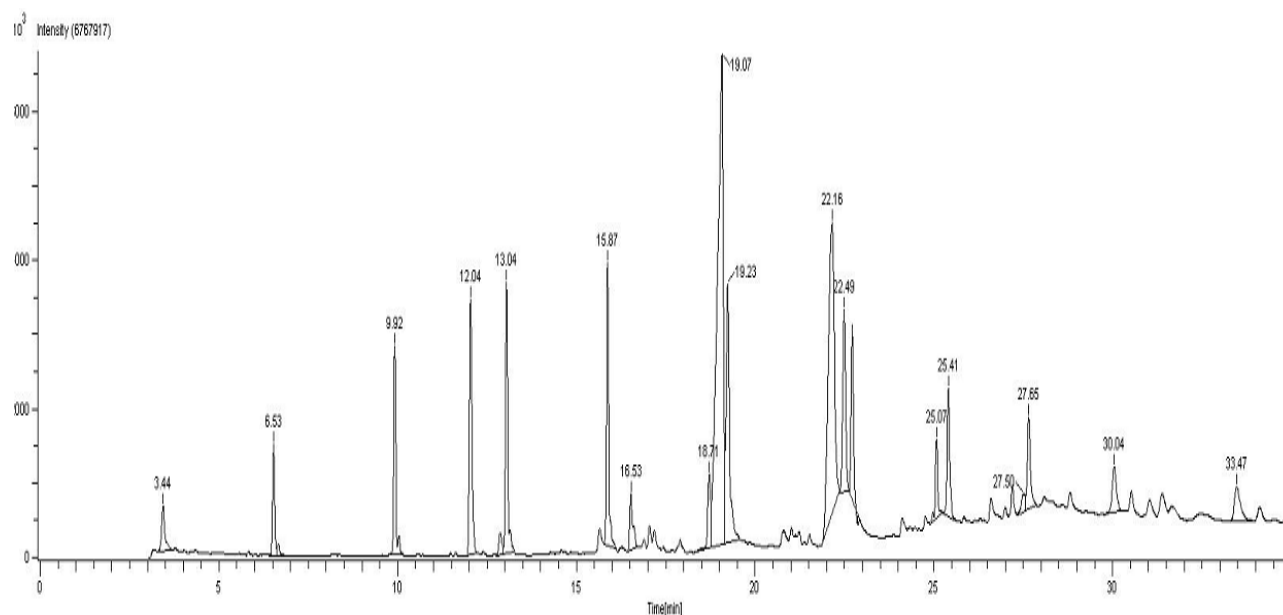


Table S1: Compounds identified in the Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Roots

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	9.92	1-Tetradecene	4.19	196	C ₁₄ H ₂₈
2.	12.04	Phenol 2,4-bis(1,1-dimethylethyl)-	6.08	206	C ₁₄ H ₂₂ O
3.	13.04	1-Hexadecene	5.61	224	C ₁₆ H ₃₂
4.	15.87	3-Octadecene,(E)-	5.72	252	C ₁₈ H ₃₆
5.	16.53	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	1.60	296	C ₂₀ H ₄₀ O
6.	19.07	n-Hexadecanoic acid	25.86	256	C ₁₆ H ₃₂ O ₂
7.	19.23	1-Nonadecene	8.16	266	C ₁₉ H ₃₈
8.	22.16	9,12-Octadecadienoic acid (Z,Z)-	16.13	280	C ₁₈ H ₃₂ O ₂
9.	22.49	Octadecanoic acid	4.84	284	C ₁₈ H ₃₆ O ₂
10.	22.71	9-Eicosene, (E)-	3.62	280	C ₂₀ H ₄₀
11.	25.07	S-Indacene, 1,2,3,5,6,7-hexahydro-1,1,5,5-tetramethyl-4,8-bis(3-methylbutyl)-	1.80	354	C ₂₆ H ₄₂
12.	27.50	3',8,8'-Trimethoxy -3-piperidyl-2,2'-binaphthalene-1.1',4,4'-tetrone	0.59	487	C ₂₈ H ₂₅ NO ₇
13.	27.65	Cis-13-Eicosenoic acid	2.64	310	C ₂₀ H ₃₈ O ₂

Figure S2: Chromatogram of Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Roots

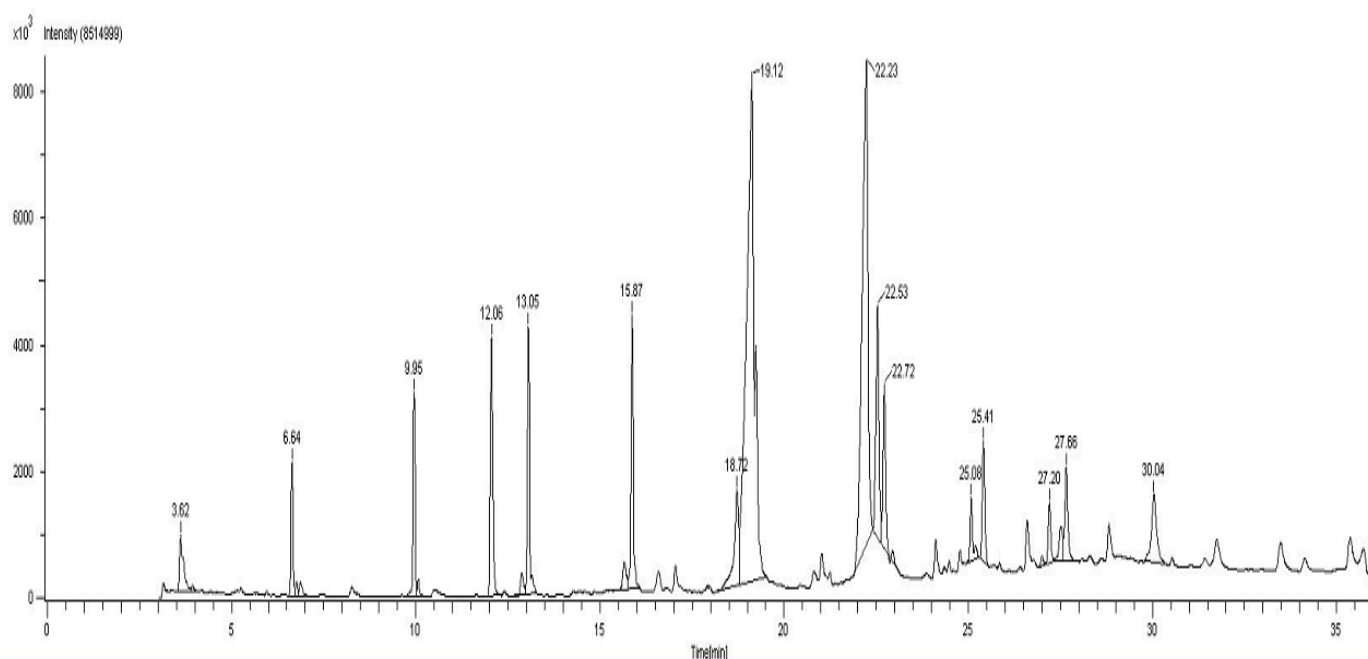


Table S2: Compounds identified in the Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Roots.

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	3.62	1-Decene	1.71	140	C ₁₀ H ₂₀
2.	6.64	1-Dodecene	2.13	168	C ₁₂ H ₂₄
3.	12.06	Phenol,2,4-bis[1,1-dimethylethyl]-	4.99	206	C ₁₄ H ₂₂ O
4.	13.05	1-Hexadecene	4.60	224	C ₁₆ H ₃₂
5.	15.87	1-Hexadecene	5.01	224	C ₁₆ H ₃₂
6.	19.12	n-Hexadecanoic acid	31.21	256	C ₁₆ H ₃₂ O ₂
7.	22.23	Oleic acid	21.59	282	C ₁₈ H ₃₄ O ₂
8.	22.53	Octadecanoic acid	5.38	284	C ₁₈ H ₃₆ O ₂
9.	22.72	1-Docosene	3.26	308	C ₂₂ H ₄₄
10.	25.08	S-Indacene, 1,2,3,5,6,7-hexahydro-1,1,5,5-tetramethyl-4,8-bis(3-methylbutyl)-	1.34	354	C ₂₆ H ₄₂
11.	25.41	1-Docosene	2.39	308	C ₂₂ H ₄₄
12.	27.66	Octatriacontyl pentafluoropropionate	2.19	696	C ₄₁ H ₇₇ F ₅ O ₂

Figure S3: Chromatogram of Ethanol extract of *Neptunia triquetra* (Vahl) Benth. Roots

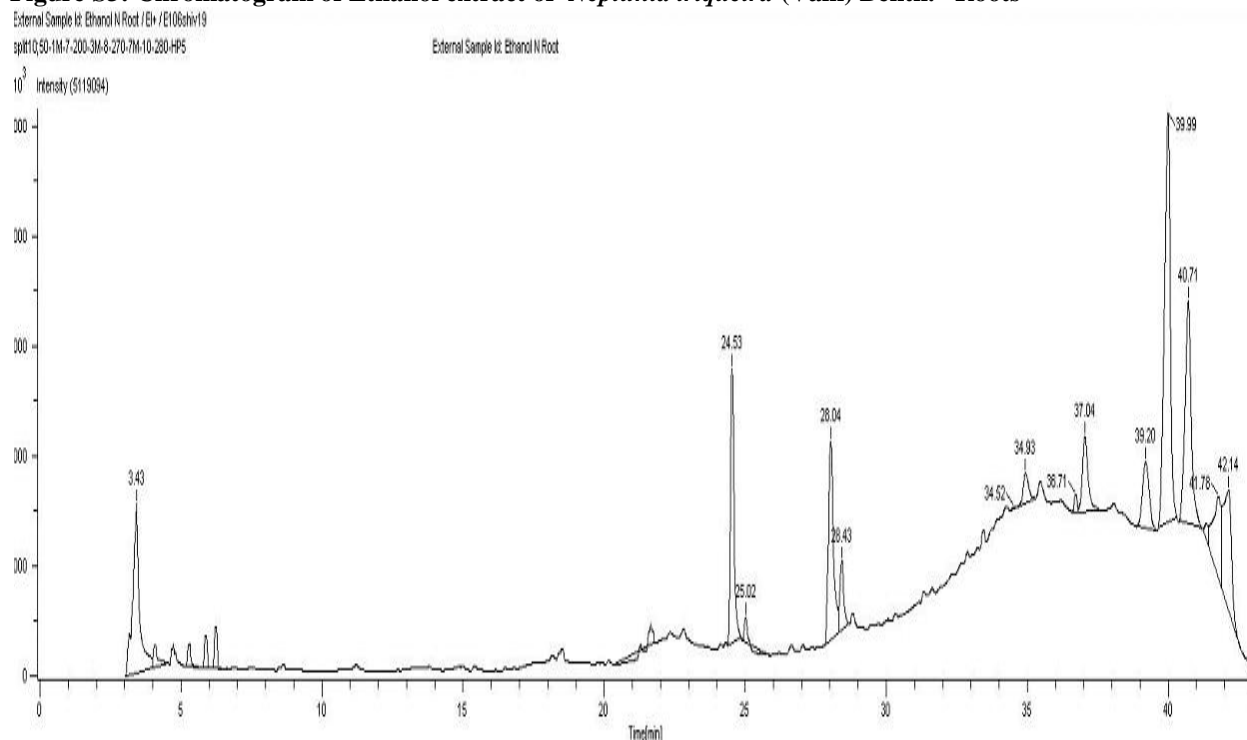


Table S3: Compounds identified in the Ethanol extract of *Neptunia triquetra* (Vahl) Benth. Roots.

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	5.31	1,3-Dioxane,4,4-dimethyl-	0.67	116	C ₆ H ₁₂ O ₂
2.	6.25	Butane,1,1-diethoxy-3-methyl-	1.11	160	C ₉ H ₂₀ O ₂
3.	8.62	Propane,1,1,3-triethoxy	0.24	176	C ₉ H ₂₀ O ₃
4.	18.52	Hexadecene	0.46	226	C ₁₆ H ₃₄
5.	21.65	1-Hexadecanol,2-methyl-	0.63	256	C ₁₇ H ₃₆ O
6.	25.02	Hexadecanoic acid,ethyl ester	0.37	284	C ₁₈ H ₃₆ O ₂
7.	28.04	Oleic acid	9.70	282	C ₁₈ H ₃₄ O ₂
8.	37.04	Stigmasterol	4.09	412	C ₂₉ H ₄₈ O
9.	39.20	Tricyclo[20.8.0.0(7,16)]triacontane,1(22),7(16)-diepoxy-	4.27	444	C ₃₀ H ₅₂ O ₂
10.	39.99	Scandenone	2.29	404	C ₂₅ H ₂₄ O ₅
11.	40.71	3,3'-Dimethyl-1'-hydroxy-5,8-dimethoxy-2,2'-binaphthalene-1,4,5',8'-tetrone	13.78	418	C ₂₄ H ₁₈ O ₇
12.	42.14	24,25-Dihydroxyvitamin D	9.28	416	C ₂₇ H ₄₄ O ₃

Figure S4: Chromatogram of Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Stem

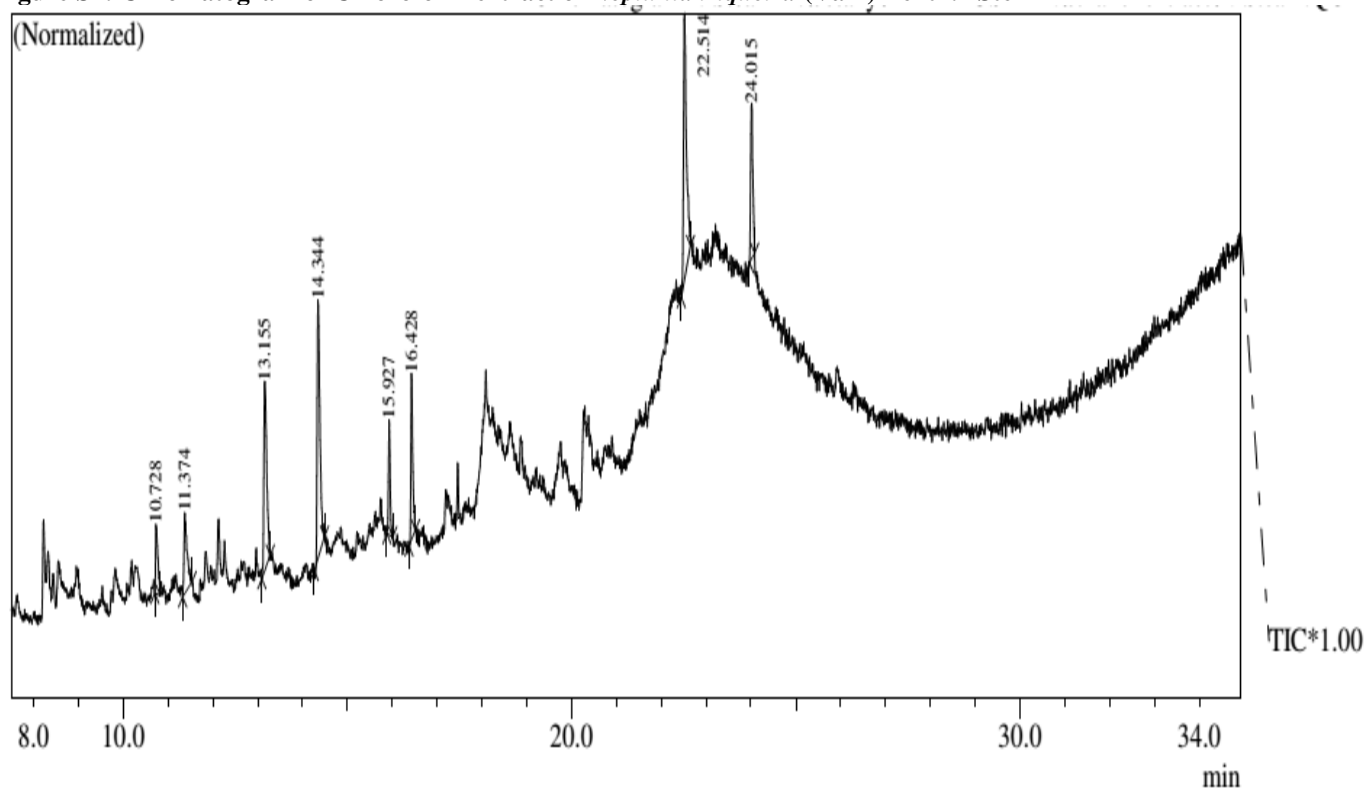


Table S4: Compounds identified in the Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Stem.

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	10.728	1-Butylpyrrolidine	4.95	127	C ₈ H ₁₇ N
2.	11.374	2,4,5-Trihydroxypyrimidine	7.50	128	C ₆ H ₈ O ₃
3.	13.155	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	15.73	144	C ₆ H ₈ O ₄
4.	14.344	2,3-dihydrobenzofuran (Dihydrocoumarone)	21.99	120	C ₈ H ₈ O
5.	15.927	4-Hydroxy-2-methylacetophenone	5.80	150	C ₉ H ₁₀ O ₂
6.	16.428	Phenol, 2,6-dimethoxy-	9.19	154	C ₈ H ₁₀ O ₃
7.	22.514	Phenol, 4-propoxy-	24.65	152	C ₉ H ₁₂ O ₂
8.	24.015	3-Butylindolizidine	10.20	181	C ₁₂ H ₂₃ N

Figure S5: Chromatogram of Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Stem

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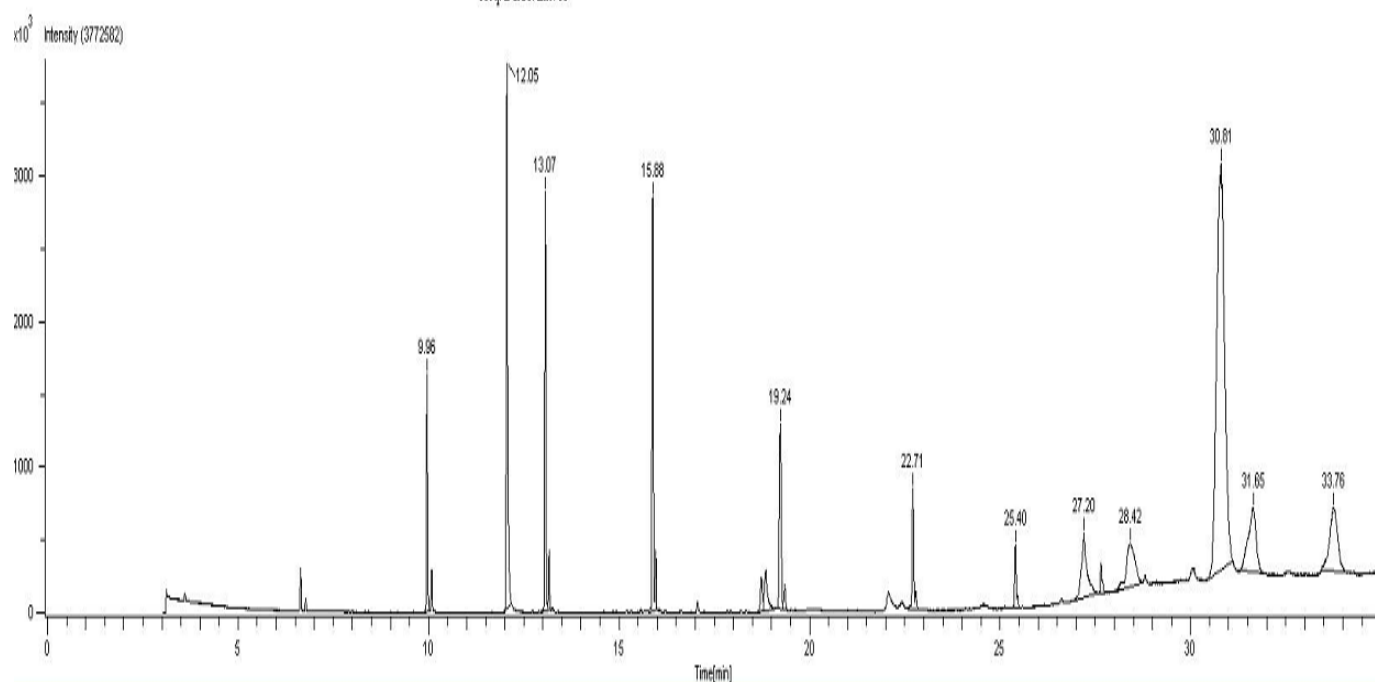


Table S5: Compounds identified in the Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Stem

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	12.05	Phenol,2,4-bis[1,1-dimethylethyl]-	9.80	206	C ₁₄ H ₂₂ O
2.	15.88	1-Nonadecene	6.74	266	C ₁₉ H ₃₈
3.	18.85	n-Hexadecanoic acid	1.56	256	C ₁₆ H ₃₂ O ₂
4.	27.20	Campesterol	4.30	400	C ₂₈ H ₄₈ O
5.	28.42	Stigmasterol	4.80	412	C ₂₉ H ₄₈ O
6.	30.81	γ-Sitosterol	40.15	414	C ₂₉ H ₅₀ O
7.	31.65	α-Amyrin	6.60	426	C ₃₀ H ₅₀ O
8.	33.76	Cycloartenol acetate	6.45	468	C ₃₂ H ₅₂ O ₂

Figure S6: Chromatogram of Ethanol extract of *Neptunia triquetra* (Vahl) Benth. Stem

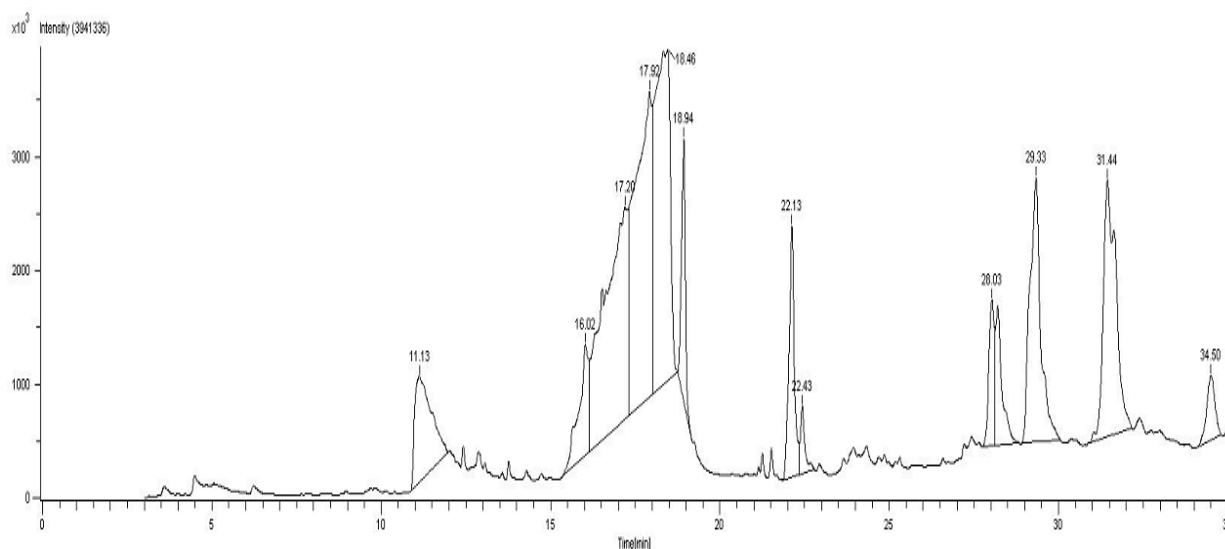


Table S6: Compounds identified in the Ethanol extract of *Neptunia triquetra* (Vahl) Benth. stem

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	4.50	1,2,3-Benzenetriol	0.76	126	C ₆ H ₆ O ₃
2.	11.13	Pyrogallol	5.94	126	C ₆ H ₆ O ₃
3.	16.02	Desulphosinigrin	3.71	279	C ₁₀ H ₁₇ NO ₆ S
4.	17.20	3-O-Methyl-d-glucose	17.72	194	C ₇ H ₁₄ O ₆
5.	18.46	3-O-Methyl-d-glucose	17.08	194	C ₇ H ₁₄ O ₆
6.	18.94	n-Hexadecanoic acid	3.46	256	C ₁₆ H ₃₂ O ₂
7.	21.52	Phytol	0.24	296	C ₂₀ H ₄₀ O
8.	22.13	Linolenic acid	4.49	278	C ₁₈ H ₃₀ O ₂
9.	22.43	Octadecanoic acid	1.01	284	C ₁₈ H ₃₆ O ₂
10.	29.33	Stigmasterol	9.80	412	C ₂₉ H ₄₈ O
11.	31.44	3,3'-Dimethyl-1'-hydroxy-5,8-dimethoxy-2,2'-binaphthalene-1,4,5',8'-tetrone	11.09	418	C ₂₄ H ₁₈ O ₇
12.	31.64	γ-Sitosterol	8.88	414	C ₂₉ H ₅₀ O
13.	34.50	Lupeol	1.80	426	C ₃₀ H ₅₀ O

Figure S7: Chromatogram of Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Leaves

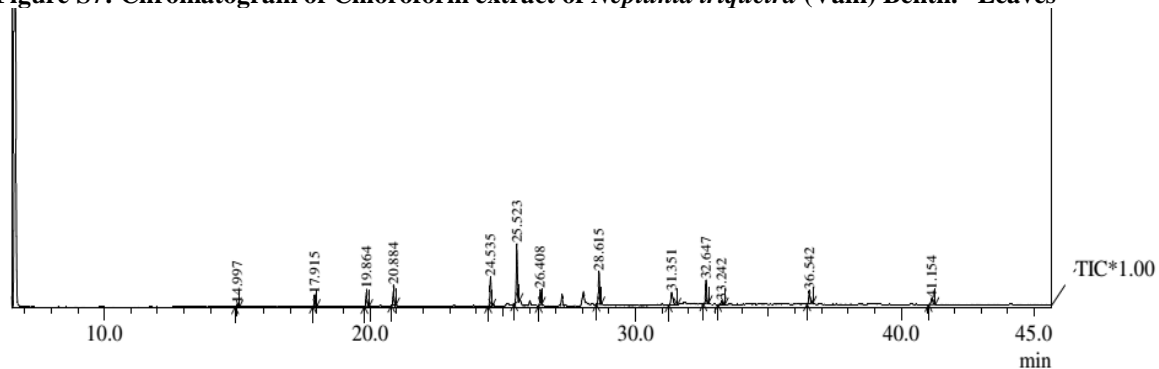


Table S7: Compounds identified in the Chloroform extract of *Neptunia triquetra* (Vahl) Benth. Leaves

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	14.997	1-Dodecanol	1.02	186	C ₁₂ H ₂₆ O
2.	17.915	1-Tetradecano	3.88	214	C ₁₄ H ₃₀ O
3.	19.864	Phenol, 3,5-bis(1,1-dimethylethyl)-	7.03	206	C ₁₄ H ₂₂ O
4.	20.884	1-Pentadecene	6.64	210	C ₁₅ H ₃₀
5.	24.535	1-Octadecanol	11.56	270	C ₁₈ H ₃₈ O
6.	25.523	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	22.27	296	C ₂₀ H ₄₀ O
7.	26.408	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	5.98	296	C ₂₀ H ₄₀ O
8.	28.615	1-Heptadecanol	12.40	256	C ₁₇ H ₃₆ O
9.	31.351	Dihydrogeraniol	8.74	156	C ₁₀ H ₂₀ O
10.	32.647	Behenic alcohol	8.76	326	C ₂₂ H ₄₆ O
11.	33.242	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-	1.83	152	C ₁₀ H ₁₆ O
12.	36.542	1-Nonadecene	6.14	266	C ₁₉ H ₃₈
13.	41.154	1-Heneicosyl formate	3.76	340	C ₂₂ H ₄₄ O ₂

Figure S8: Chromatogram of Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Leaves

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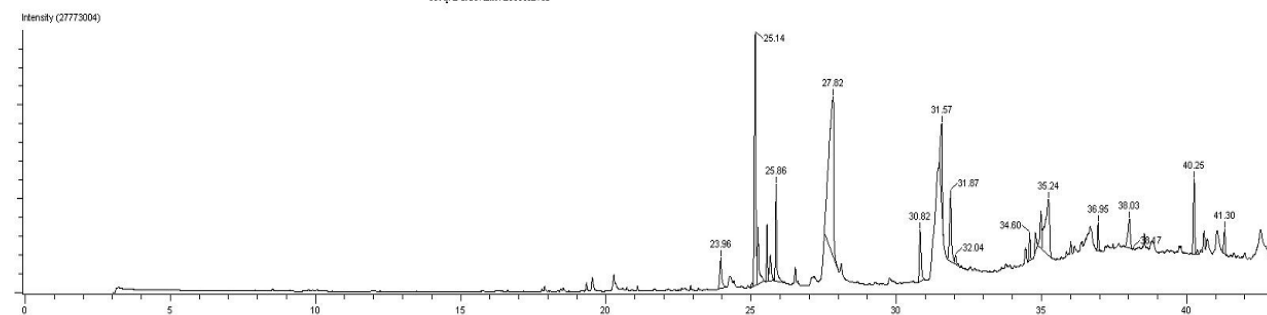


Table S8: Compounds identified in the Dichloromethane extract of *Neptunia triquetra* (Vahl) Benth. Leaves.

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	17.89	Humelene	0.46	204	C ₁₅ H ₂₄
2.	19.53	2(4H)-Benzofuranone, 5,6,7,7a-terahydro-4,4,7a-trimethyl-(R)-	0.76	180	C ₁₁ H ₁₆ O ₂
3.	20.28	Dodecanoic acid	1.00	200	C ₁₂ H ₂₄ O ₂
4.	23.95	Tetradecanoic acid	1.28	228	C ₁₄ H ₂₈ O ₂
5.	25.14	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	10.10	296	C ₂₀ H ₄₀ O
6.	25.24	2-Pentadecanone, 6,10,14-trimethyl-	1.86	268	C ₁₈ H ₃₆ O
7.	25.56	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	2.37	296	C ₂₀ H ₄₀ O
8.	27.80	n-Hexadecanoic acid	26.59	256	C ₁₆ H ₃₂ O ₂
9.	30.83	Phytol	2.35	296	C ₂₀ H ₄₀ O
10.	31.54	Linolenic acid	18.79	278	C ₁₈ H ₃₀ O ₂
11.	31.86	Octadecanoic acid	3.28	284	C ₁₈ H ₃₆ O ₂
12.	38.02	Octadecane, 3-ethyl-5-(2-ethylbutyl)	2.02	366	C ₂₆ H ₅₄
13.	40.60	Squalene	1.58	410	C ₃₀ H ₅₀
14.	42.55	Octadecane, 3-ethyl-5-(2-ethylbutyl)	3.25	366	C ₂₆ H ₅₄

Figure S9: Chromatogram of Ethanol extract of *Neptunia triquetra* (Vahl) Benth. Leaves

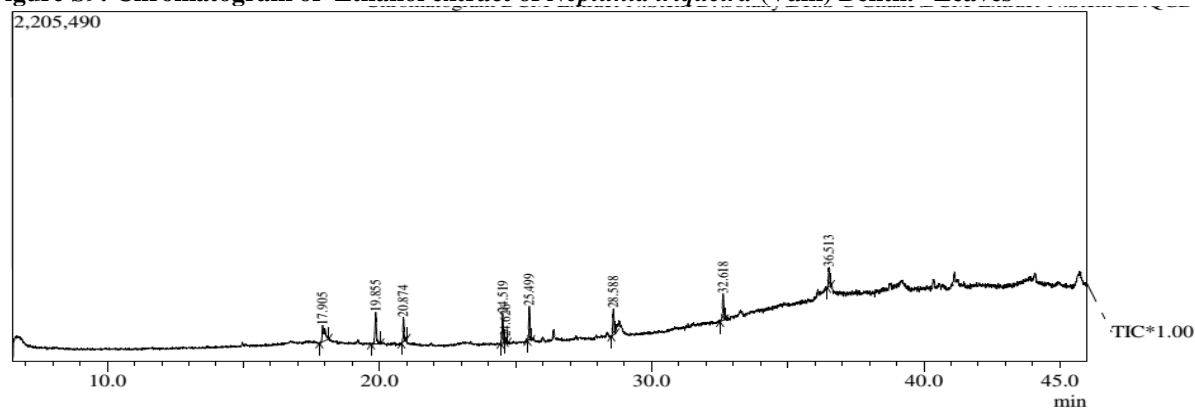
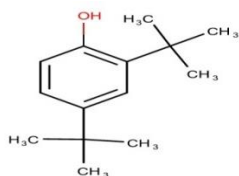


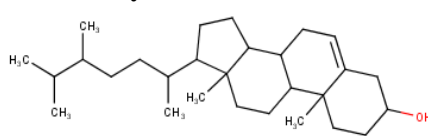
Table S9: Compounds identified in the Ethanol extract of *Neptunia triquetra* (Vahl) Benth. Leaves.

S. No.	RT	Name of Compound	Peak Area %	MW	MF
1.	17.905	1-Heptadecene	14.60	238	C ₁₇ H ₃₄
2.	19.855	Phenol, 2,4-bis(1,1-dimethylethyl)-	15.91	206	C ₁₄ H ₂₂ O
3.	20.874	1-Heptadecanol	8.95	256	C ₁₇ H ₃₆ O
4.	24.519	1-Octadecanol	12.39	270	C ₁₈ H ₃₈ O
5.	24.626	Norphytan	1.65	268	C ₁₉ H ₄₀
6.	25.499	3,7,11,15-Tetramethyl-2-hexadecen-1-ol	15.14	296	C ₂₀ H ₄₀ O
7.	28.588	1-Nonadecene	11.23	266	C ₁₉ H ₃₈
8.	32.618	Behenic alcohol	12.01	326	C ₂₂ H ₄₆ O
9.	36.513	1-Eicosanol	8.10	298	C ₂₀ H ₄₂ O

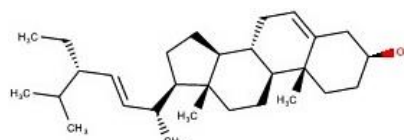
Molecular structures of Identified Secondary Metabolites



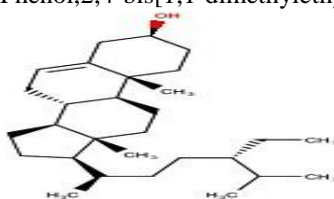
Phenol, 2,4-bis[1,1-dimethylethyl]-



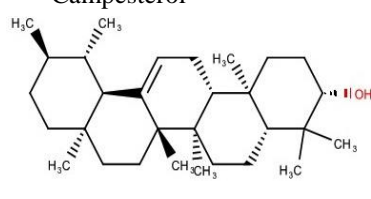
Campesterol



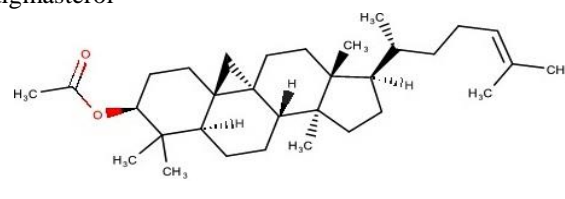
Stigmasterol



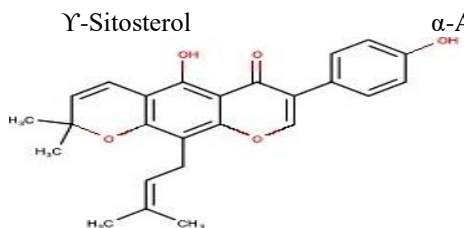
γ-Sitosterol



α-Amyrin

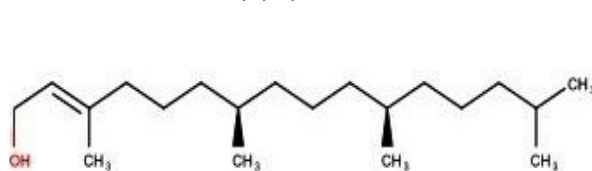


Cycloartenol acetate

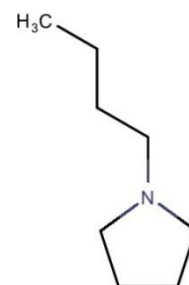


Scandone (Warangalone)

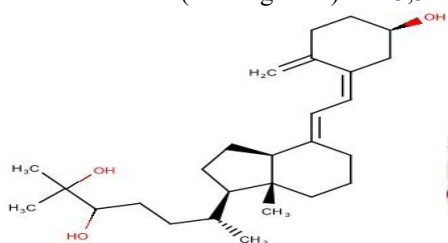
3,3'-Dimethyl-1'-hydroxy-5,8-dimethoxy-2,2'-binaphthalene-1,4,5',8'-tetrone



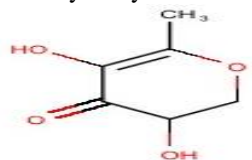
3,7,11,15-Tetramethyl-2-hexadecen-1-ol



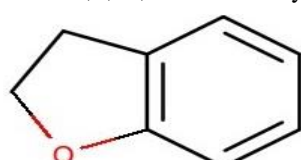
1-Butylpyrrolidine



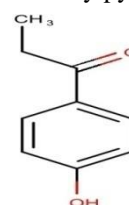
24,25-Dihydroxyvitamin D



4H-Pyran-4-one, 2,3-dihydro, -3,5-dihydroxy-6-methyl



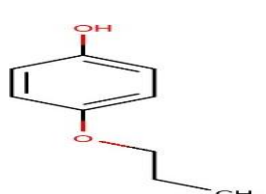
Benzofuran, 2,3-dihydro-



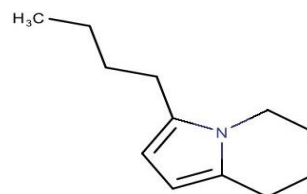
4-Hydroxy-2-methylacetophenone



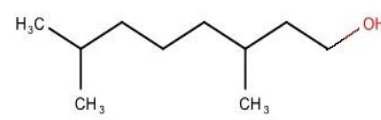
Phenol, 2,6-dimethoxy-



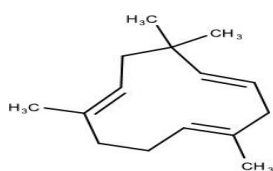
Phenol, 4-propoxy-



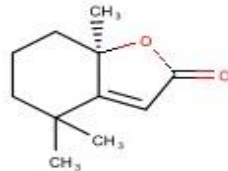
3-Butylindolizidine



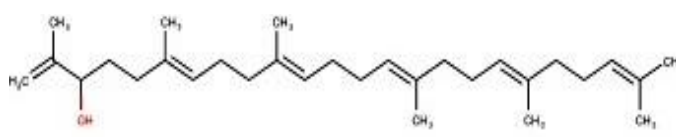
Dihydrogeraniol



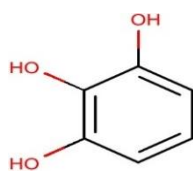
α-Caryophyllene (Humelene)



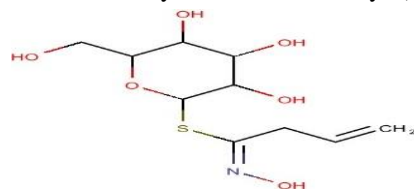
2(4H)-Benzofuranone 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-(R)-



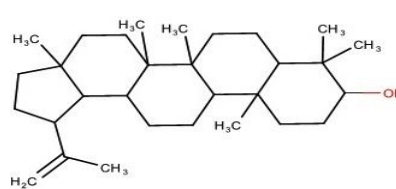
Squalene



Pyrogallol



Desulphosinigrin



Lupeol