

TITLE

Validating potent anti-inflammatory and anti-rheumatoid properties of *Drynaria quercifolia* rhizome methanolic extract through *in vitro*, *in vivo*, *in silico* and GC-MS-based profiling.

Authors:

Debabrata Modak¹, Subhashis Paul¹, Sourav Sarkar¹, Subarna Thakur² and Soumen Bhattacharjee^{1*}.

¹Cell and Molecular Biology Laboratory, Department of Zoology, University of North Bengal, Darjeeling 734013, West Bengal, India.

²Department of Bioinformatics, University of North Bengal, Darjeeling 734013, West Bengal, India.

Title: Additional file 2

Description: List of compounds identified in GC-MS analysis with their chemical class and biological properties.

Sl No.	Compound Name with formula	Chemical class	Molecular Weight (kDa); Retention Time (second)	Area%	SI	Biological Properties with Reference
1.	Silane, ethenylethoxydimethyl- [C ₆ H ₁₄ OSi ₂]	Group 14 hydride	130; 8.227	1.63	78	Not reported
2.	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl- [C ₆ H ₈ O ₄]	Pyranone	144; 9.357	1.11	94	Anti-proliferative and pro-apoptotic [1],Antioxidant [2], Modulate autonomic nerve activity in Rat model [3]
3.	Catechol [C ₆ H ₆ O ₂]	Benzenediols	110; 10.333	5.07	95	Antimicrobial [4]
4.	5-Hydroxymethylfurfural [C ₆ H ₆ O ₃]	Furans	126; 10.743	1.32	90	Antioxidant and Antiproliferative [5], Inhibitory effect on the sickling of red blood cells [6], Anti-allergic (Type I allergic Diseases [7],Anti-inflammatory [8]
5.	Benzeneacetic acid [C ₈ H ₈ O ₂]	Monocarboxylic acid containing a phenyl group	136; 11.050	0.27	85	Antimicrobial [9], Anti-inflammatory [10], Derivatives of phenylacetic acids [11]
6.	Beta.-d-Ribopyranoside, methyl, 3-acetate [C ₈ H ₁₄ O ₆]	D-ribopyranose	206; 14.807	0.40	78	Not reported
7.	Dodecanoic acid [C ₁₂ H ₂₄ O]	Saturated fatty acid	200; 15.083	0.50	95	Not reported
8.	Benzenepropanoic acid, 4-hydroxy-, methyl ester [C ₁₀ H ₁₂ O ₃]	Phenyl <u>propanoids</u>	180; 15.377	0.34	85	Not reported

9.	1,3,4,5-tetrahydroxycyclohexane carboxylic acid [C ₇ H ₁₂ O ₆]	Cyclitol and cyclohexanecarboxylic acid	192; 16.780	4.44	85	Not reported
10.	Tetradecanoic acid [C ₁₄ H ₂₈ O ₂]	Saturated fatty acid	228; 17.367	0.88	95	Larvicidal and repellent [12]
11.	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester [C ₁₆ H ₂₂ O ₄]	Benzoic acid esters	278; 18.400	1.14	97	Not reported
12.	n-Pentadecanol [C ₁₅ H ₃₂ O]	Saturated long-chain fatty alcohol	228; 18.590	0.29	97	Antimicrobial [13]
13.	Hexadecanoic acid, methyl ester [C ₁₇ H ₃₄ O ₂]	Saturated fatty acid	270; 19.017	0.91	96	Anti-inflammatory, Anti microbial, Antioxidant [14,15]
14.	2-hydroxycyclopentadecanone [C ₁₅ H ₂₈ O ₂]	Cyclopentadecanone	240; 19.233	0.47	85	Not reported
15.	Dibutyl phthalate [C ₁₆ H ₂₂ O ₄]	Phthalates	278; 19.363	0.17	95	Antimicrobial, Anti-inflammatory [16,17]
16.	n-Hexadecanoic acid [C ₁₆ H ₃₂ O ₂]	Saturated fatty acid	256; 19.507	7.30	96	Anti-bacterial, Anti-fungal [18]
17.	Alpha.-D-Glucopyranoside, methyl [C ₇ H ₁₄ O ₆]	Monosaccharide	194; 20.203	0.79	84	Growth inhibitory effect on mammalian cells and parasites [19]
18.	n-Nonadecanol-1 [C ₁₉ H ₄₀ O]	Long-chain fatty alcohols	284; 20.593	1.11	97	Antimicrobial, Cytotoxic activity [20]
19.	9,12-Octadecadienoic acid (Z,Z)-, methyl ester [C ₁₉ H ₃₄ O ₂]	Polyunsaturated Omega-6 trans fatty acid (TFA)	294; 20.657	0.58	95	Anti-inflammatory, Anti-cancer [21,22]
20.	6-Octadecenoic acid, methyl ester, (Z)- [C ₁₉ H ₃₆ O ₂]	Monounsaturated omega-12 fatty acid	296; 20.717	0.52	93	Not reported
21.	cis-9-Hexadecenal [C ₁₆ H ₃₀ O]	Monounsaturated omega-7 fatty acid	238; 21.167	6.04	91	Antimicrobial [23]
22.	Octadecanoic acid [C ₁₈ H ₃₆ O ₂]	Saturated fatty acid	284; 21.347	0.80	93	Antimicrobial [24]
23.	4,8,12,16-Tetramethylheptadecan-4-olide [C ₂₁ H ₄₀ O ₂]	Long-chain methyl-branched fatty acid	324; 22.950	0.23	96	Not reported
24.	1-Heptacosanol [C ₂₇ H ₅₆ O]	Long-chain primary fatty alcohol	396; 24.093	0.47	95	Antimicrobial [20]
25.	Hexadecanoic acid, 2-	2-monoglyceride	330;	2.32	92	Not reported

	hydroxy-1-(hydroxymethyl)ethyl ester [C ₁₉ H ₃₈ O ₄]		24.273			
26.	Bis(2-ethylhexyl) phthalate [C ₂₄ H ₃₈ O ₄]	Diester of phthalic acid and the branched-chain 2-ethylhexanol	390; 24.407	0.30	96	Antimicrobial, Cytotoxic activity [25]
27.	9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-hydroxymethyl)ethyl ester [C ₂₁ H ₃₈ O ₄]	2-monoglyceride	354; 25.690	3.98	91	Not reported
28.	Squalene [C ₃₀ H ₅₀]	Triterpene	410; 26.753	0.76	97	Anti inflammatory, Anticancer, Antioxidant [26,27,28,29,30]
29.	Gamma.-Tocopherol [C ₂₈ H ₄₈ O ₂]	Tocopherol	416; 29.767	0.40	94	Potent Anti-inflammatory, Anti-cancer [31,32,33,34]
30.	Vitamin E [C ₂₉ H ₅₀ O ₂]	Tocopherol	430; 31.090	2.01	95	Anti-inflammatory, Anti-cancer, Antioxidant, Immunomodulatory, Wound healing [35,36,37,38]
31.	A'-neogammacer-22(29)-ene [C ₃₀ H ₅₀]	Triterpene	410; 31.797	0.59	83	Not reported
32.	1-phenanthrenecarboxylic acid, 7-ethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,4a,7-trimethyl-, methyl Ester, [C ₂₁ H ₃₄ O ₂]	Fatty acid ester	318; 32.357	6.07	65	Not reported
33.	Ergost-5-en-3-ol, (3.beta.,24r) [C ₂₈ H ₄₈ O]	Steroid	400; 33.110	1.32	93	Not reported
34.	Cholest-5-en-3-ol, 4,4-dimethyl-, (3.beta.) [C ₂₉ H ₅₀ O]	Steroid	414; 33.703	4.17	82	Not reported
35.	Ergosta-8,24(28)-dien-3-ol, 4,14-dimethyl-, (3.beta.,4.alpha.,5.alpha.)-[C ₃₀ H ₅₀ O]	3beta-sterol	426; 34.603	3.07	86	Not reported
36.	Stigmast-5-en-3-ol, (3.beta.) [C ₂₉ H ₅₀ O]	Sterol	414; 35.180	4.98	81	Immunomodulatory,

						Apoptotic, Anti-proliferative [39,40]
37.	Cholest-5-en-3-ol, 4,4-dimethyl-, (3.beta.)-[C ₂₉ H ₅₀ O]	3beta-sterol	414; 36.577	0.44	78	Antilisterial activity [41]
38.	9,19-Cyclolanost-24-en-3-ol, (3.beta.)-[C ₃₀ H ₅₀ O]	Triterpenoid	426; 37.313	1.34	91	Not reported
39.	9,19-Cyclolanost-25-en-3-ol, 24-methyl-, (3.beta.,24S)-[C ₃₁ H ₅₂ O]	Triterpenoid	440; 38.407	0.65	78	Not reported
40.	(1,5-dimethyl-hexyl)-3a,10,10,12b-tetramethyl-1,2,3,3a,4,6,8,9,10,10a,11,12,12a,12b-tetradecahydro-benzo[4,5]cyclohepta[1,2-e]inde [C ₃₀ H ₅₀ O]	Triterpenoid	410; 38.833	1.34	82	Not reported
41.	Cyclopropa[5,6]-33-norgorgostan-3-ol, 3',6-dihydro-, (3.beta.,5.beta.,6.alpha.,22.xi.,23.xi.)- [C ₃₀ H ₅₀ O]	Triterpenoid	426; 39.143	3.41	79	Not reported
42.	9,19-Cyclolanostan-3-ol, 24-methylene-, (3.beta.)-[C ₃₁ H ₅₂ O]	Triterpenoid	440; 40.447	0.89	83	Not reported
43.	5-(7a-Isopropenyl-4,5-dimethyl-octahydroinden-4-yl)-3-methyl-pent-2-en-1-ol [C ₂₀ H ₃₄ O]	Triterpenoid	290; 41.147	1.29	80	Not reported
44.	9,19-cyclolanostan-3-ol, 24-methylene-, (3.beta.)-[C ₃₁ H ₅₂ O]	Triterpenoid	440; 41.843	0.78	90	Not reported
44.	9,19-Cyclolanostan-3-ol, 24-methylene-, (3.beta.)-[C ₃₁ H ₅₂ O]	Triterpenoid	440; 42.387	1.49	91	Not reported
45.	Lanost-8-ene-3,22,23-triol, 24-methylene-, 22-acetate, (3.beta.,22r,23s)-[C ₃₃ H ₅₄ O ₄]	Triterpenoid	514; 44.267	0.98	56	Not reported
46.	9,19-Cyclolanostan-3-ol, 24-methylene-, (3.beta.)-[C ₃₁ H ₅₂ O]	Triterpenoid	440; 44.943	0.80	83	Not reported
47.	9,19-cycloergost-24(28)-en-3-ol, 4,14-dimethyl-, (3.beta.,4.alpha.,5.alpha.) [C ₃₀ H ₅₀ O]	Triterpenoid	426; 48.603	0.78	79	Not reported

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