

Non-targeted secondary metabolite profile study for deciphering the cosmeceutical potential of red marine macro alga *Jania rubens* - An LCMS based approach

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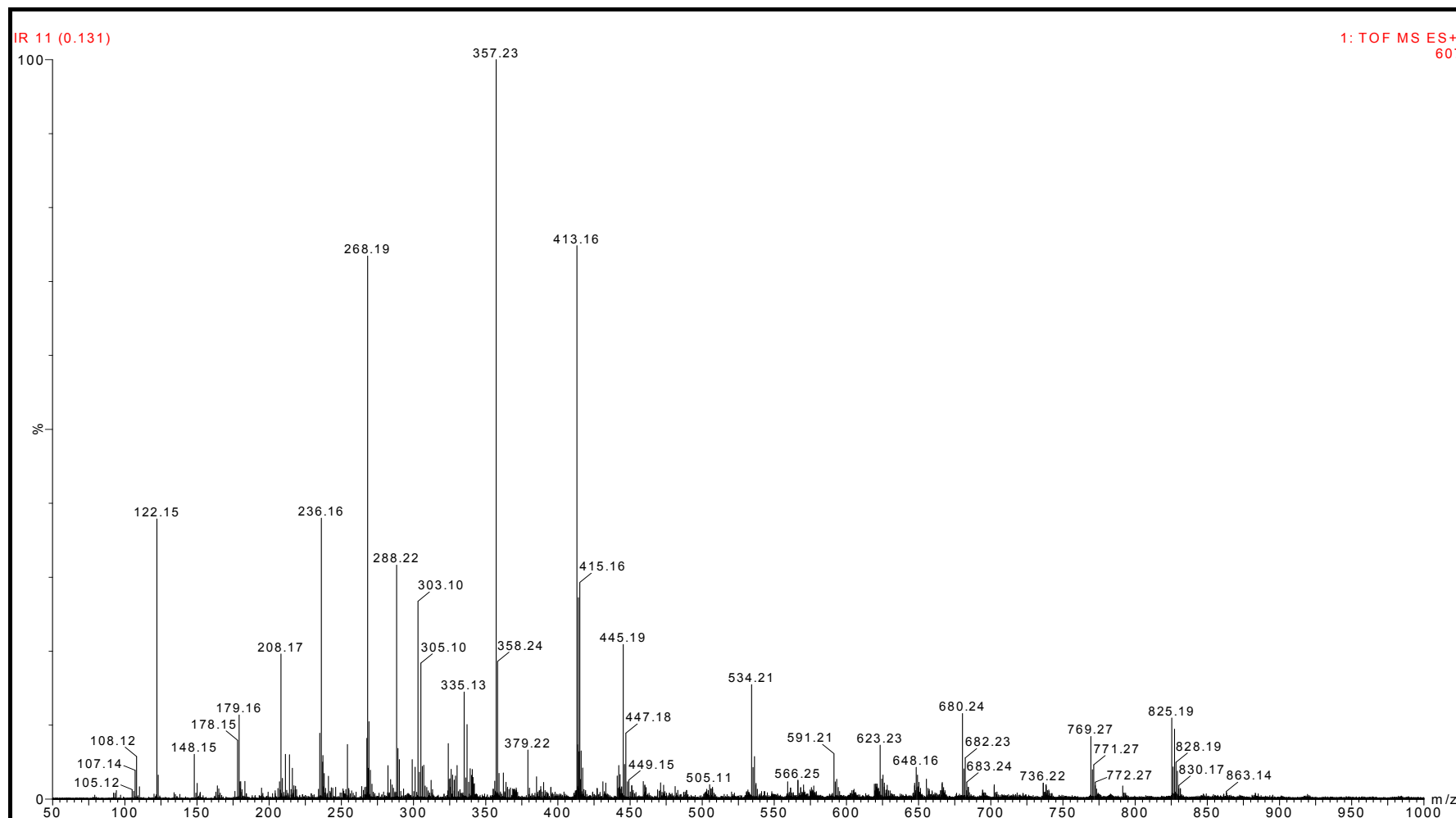


Figure S1. Metabolite Profile of *J. rubens* extract using LCMS (ESI positive mode).

Table S1: Putative metabolites identified in *J.rubens* extract and their possible function/application/role/importance.

Name of the probable/putative metabolites	Δ PPM	m/z	Formula	Metlin Id. No.	LMID/KEGG/HMDB	Category/Class/ Sub class	Probable Function/Role/Importance/Utility
γ coniceine	21	108.12	C ₈ H ₁₅ N	68145	KEGG (C10138)	Alkaloid	Biosynthesis of plant secondary metabolites. Biosynthesis of alkaloids derived from terpenoid and polyketide.
Berberrubin	17	305.1	C ₁₉ H ₁₆ NO ₄	86846	HMDB30266	Alkaloid	Berberrubine is found in fruits. Berberrubine is an alkaloid from Berberis vulgaris (barberry) Berberrubine has been found to exhibit anti-fungal function.
Tsangane L3 glucoside	6	357.23	C ₁₉ H ₃₄ O ₇	95286	HMDB40824	Terpene glycosides	Potential aromatic compound.
Icaceine	4	358.24	C ₂₂ H ₃₃ NO ₄	67123	KEGG (C08689)	Diterpene-based alkaloid	Used as an anticonvulsant due to its alkaloid content.
Cubebinone	0	413.16	C ₂₃ H ₂₆ O ₈	89123	HMDB33259	Natural lignan compound	Found in herbs and spices.
8-Acetoxy-4'-methoxypinoresinol	0	413.16	C ₂₃ H ₂₆ O ₈	89136	HMDB33277	Furanoid lignans	Aromatic heteropolycyclic compound.

Sesartemin	0	413.16	C ₂₃ H ₂₆ O ₈	68654	KEGG (C10884)	Phenylpropanoid, Lignan	Aromatic heteropolycyclic compounds. This compound belongs to the class of chemical entities known as furanoid lignans. These are lignans with a structure that contains either a tetrahydrofuran ring, a furan ring, or a furofuan ring system, that arises from the joining of the two phenylpropanoid units.
(-)-Medicocarpin	25	415.15	C ₂₂ H ₂₄ O ₉	64291	KEGG (C16223)	Flavonoid	It is found in Alfalfa.
Zizybeoside I	25	415.15	C ₁₉ H ₂₈ O ₁₁	71779	KEGG (C17564)	Crude drug	Major component of natural products. Found in Jujube seed.
Benzyl gentiobioside	25	415.15	C ₁₉ H ₂₈ O ₁₁	95899	HMDB41515	O-glycosyl compound	It is found in garden tomato. Used as a nutrient.
4'-O-Methylglucoliquiritigenin	25	415.15	C ₂₂ H ₂₄ O ₉	94470	HMDB39927	Flavonoid-7-o-glycosides	It is found in herbs and spices.
Trichocarposide	25	415.15	C ₂₂ H ₂₄ O ₉	87895	HMDB31723	Phenolic glycoside	Aromatic coumaric acid ester derivative.
Agecorynin C	25	415.15	C ₂₂ H ₂₄ O ₉	49925	KEGG (C14942)	Flavonoid	It is found to be present in <i>Ageratum conyzoides</i> that plays a role in traditional medicine. It is widely used externally to treat skin diseases, wounds (both disinfection and homoeostasis), ulcers and boils; internally as febrifuge and to treat diarrhea and hemorrhages.
5,6,7,8,3',4',5'-Heptamethoxyflavone	25	415.15	C ₂₂ H ₂₄ O ₉	49916	KEGG (C14953)	Flavonoid (Polymethoxxygenated flavone)	Antiprotozoal, Insecticidal and allopathic.

6-O-Methylarmillaridin	4	445.18	C ₂₅ H ₃₁ ClO ₆	90952	HMDB35690	Melleolides and analogues, prenol lipids	Used as stabilizer, emulsifier and nutrient.
Eremopetasitenin B2	9	447.18	C ₂₄ H ₃₂ O ₇ S	87269	HMDB30901	Eremophilanolides (Naphthofuran)	It is found in green vegetables. Used as a stabilizer, surfactant, emulsifier and nutrient.
Eremosulphoxinolide A	9	447.18	C ₂₄ H ₃₂ O ₇ S	95915	HMDB41532	Terpene lactones	It is found in green vegetables. Used as a stabilizer, surfactant, emulsifier and nutrient.
Agnuside	11	449.15	C ₂₂ H ₂₆ O ₁₁	67924	KEGG (C09765)	Glucoside	Hepatoprotective properties, anti-inflammatory, antioxidant and analgesic.
Simmondsin 2'-ferulate	23	534.21	C ₂₆ H ₃₃ NO ₁₂	90759	HMDB35475	Coumaric acid esters	Aromatic compounds containing an ester derivative of coumaric acid. Found in coffee and coffee products and constituents of jojoba seeds.
Malonylshisonin	2	825.19	C ₃₉ H ₃₈ O ₂₁	46929	KEGG C16299	Flavonoid	Anthocyanin biosynthesis pathway.
4'''-Demalonylsalvianin	2	825.19	C ₃₉ H ₃₈ O ₂₁	64254	KEGG C12641	Flavonoid	Anthocyanin biosynthesis pathway.
Maclurin 3-C-(2'',3'',6''-trigalloylglucoside)	22	863.15	C ₄₀ H ₃₂ O ₂₃	88585	HMDB32643	Hydrolysable Tannin	It is found in fruits. Its application includes that of a nutrient.
Theaflavonin	25	919.18	C ₄₃ H ₃₆ O ₂₄	94955	HMDB40453	Complex Tannin	It is found in tea. Used as a nutrient.