

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

Dhara C. Dixit^{1*}, C R K Reddy²

¹ Department of Earth & Environmental Science, Krantiguru Shyamji Krishna Verma Kachchh University, Bhuj-Kachchh, 370001, Gujarat, India;

² Discipline of Marine Biotechnology & Ecology, CSIR-Central Salt and Marine Chemicals Research Institute, Gijubhai Badheka Marg, Bhavnagar-364002, Gujarat, India; crk@csmcri.res.in

* Correspondence: dharadixit2008@gmail.com; Tel.: +91-9979090900

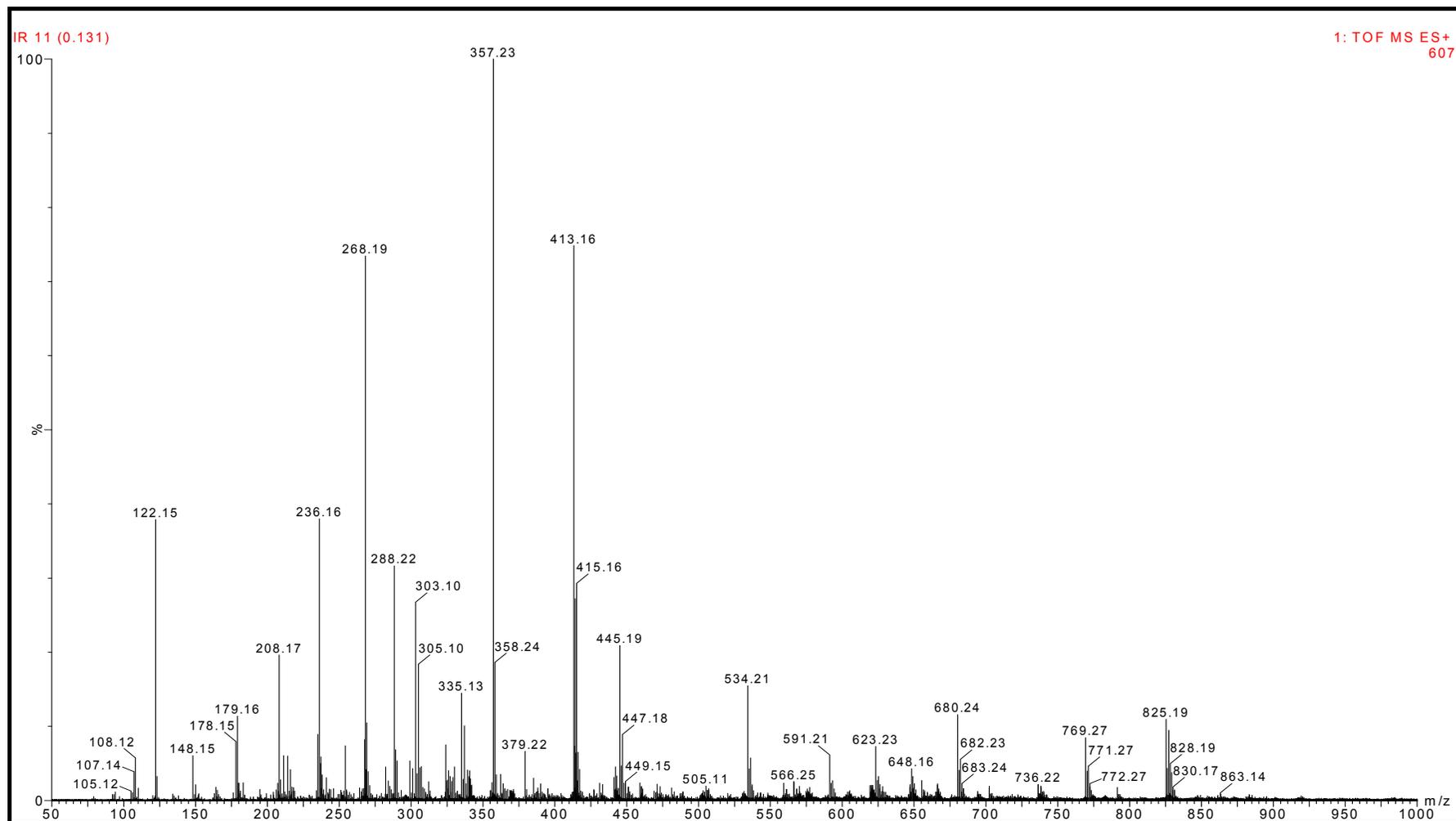


Figure S1. Metabolite Profile of *J. rubens* extract using LCMS (ESI positive mode).

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

| Name of the probable/putative metabolites | ΔPPM | 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 <i>Berberis vulgaris</i> (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 (Polymethoxygenated 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. |
| Theaflavinin | 25 | 919.18 | C ₄₃ H ₃₆ O ₂₄ | 94955 | HMDB40453 | Complex Tannin | It is found in tea. Used as a nutrient. |