**Table S1 -** Biological activities of compounds detected from *Urena lobata.*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S.No. | Name of Compounds | From other plants | Authors | Biological Activities |
| 1. 1 | 1-Hexanol, 2-ethyl- | *Vitis rotundifolia* Michx | (Deng et al., 2021) | - |
| 1. 2 | 1,2,3-Propanetriol, 1-acetate | *Punica granatum* | (Growther et al., 2012) | - |
|  | 1-Nonene, 4,6,8-trimethyl- | *Moringa concanensis* | (Balamurugan et al., 2015) | Allelochemical |
|  | 3,5-Dithiahexanol 5,5-dioxide | *Salvadora persicahadi* | (Hadi Hameed et al., 2018) | - |
|  | Nonanoic acid | Palm oil | (Aneja et al., 2005; Kamatou and Viljoen, 2017) | Anti-microbial |
|  | 1-Undecanol | *Senecio belgaumensis* | (Joshi, 2011) | Insecticidal |
|  | 1-dodecanol | *Mikania species* | (Cueto et al., 2005; Da Silva et al., 1984) | Insecticidal activity |
|  | Hexadecane; | Green macroalgae | (Shah et al., 2022) | - |
|  | hexadecanoic acid butyl ester | Green macroalgae | (Shah et al., 2022) | Anti-sickling activity |
|  | Octane 2-bromo- | Green macroalgae | (Shah et al., 2022) | - |
|  | Phenol 2,4-bis(1,1-dimethyl ethyl)- | Green macroalgae and Avocado roots | (Rangel-Sánchez et al., 2014) | Anti-microbial |
|  | 7-hexadecenoic acid methyl ester (z)- | Green macroalgae | (Gayathiri et al., 2022) | Anti-proliferative activities |
|  | Hexadecanoic acid methyl ester | Green macroalgae | (Heidary Jamebozorgi et al., 2019) | Anti-proliferative activities, anti-bacterial |
|  | Hexadecane | *Dillenia suffruticosa* | (Shah et al., 2020; Siporin and Cooney, 1976) | Inhibit glucose metabolism |
|  | Methyl stearate | *Dillenia suffruticosa* | (Nirmal et al., 2022; Shah et al., 2020) | Anti-mirbobial |
|  | Hexadecanoic acid ethyl ester | *Sargassum wightii* | (Balachandran et al., 2016) | Anit-inflammatory |
|  | (E)-9-Octadecenoic acid ethyl ester | *Nelumbo nucifera* Gaertn | (Xie et al., 2022) | Anit-inflammatory |
|  | 9,12-octadecadienoic acid (Z, Z)- methyl ester | *Eclipta alba* | (Jayaraman et al., 2022) | Anti-cancerous |
|  | 9-octadecenoic acid (Z)- methyl ester | *Senna alata L.* | (Muhammad et al., 2021) | Antibacterial |
|  | 1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester | *Nephrolepis cordifolia* | (Stroheker et al., 2005) | Anti-androgenic activity |
|  | Cyclopropaneoctanoic acid, 2-[[2-[(2-ethylcyclopropyl)methyl]cyclopropyl]methyl]-, methyl ester | *Gaillardia pulchella* Foug | (Yao et al., 2013) | - |
|  | Hexanoic acid, 2-ethyl-hexadecyl ester | Grapes | (Chang et al., 2014) | - |
|  | Heptanoic acid, 4-octyl ester | *Pyrus communis* L. | (Chen et al., 2018) | - |
|  | Methyl 12,13-tetradecadienoate | *Oroxylum indicum* (L.) Benth. Ex Kurz | (Debi and Parkash, 2020) | - |
|  | 10-Heneicosene (c,t) | *Tinospora cordifolia* | (Ebin, 2021) | - |
|  | Hexanedioic acid, bis(2-ethylhexyl) ester | *Eucalyptus granlla* | (Ge et al., 2015) | - |
|  | Propanoic acid, 3-mercapto-, dodecyl ester | *Rosmarinus officinalis* | (Manilal et al., 2021) | - |
|  | Tricosyl pentafluoropropionate | *Brassica juncea* L. | (Sharma et al., 2015) | - |
|  | Benzenepropanoic acid, 3,5-bis(1,1-dimethyl ethyl)-4-hydroxy-, methyl ester | *Brassica juncea* L. | (Gayathiri et al., 2022; Sangeet et al., 2022; Sharma et al., 2015; Sonkar, 2019) | Anti-fungal, anti-neurodegenerative disorder, anti-cancer, anti-diabetic |
|  | Diisooctyl adipate | *Pleiospermium alatum* | (Parthipan et al., 2015) | - |
|  | 3-chloropropionic acid, heptadecyl ester | *Clerodendrum colebrookianum* | (Payum, 2020) | - |
|  | cis-10-Nonadecenoic acid | *Dodonaea angustifolia* | (Revathi and Dhanaraj, 2019) | - |
|  | 9,12-Octadecadienoic acid, ethyl ester | *Stylissa carteri* | (Bashari et al., 2019) | - |
|  | Dibutyl phthalate | *Stylissa carteri* | (Bashari et al., 2019) | Antiandrogenic effects |
|  | Decanedioic acid, dibutyl ester | *Eucalyptus citriodora* | (Sahi, 2016) | - |
|  | trans-13-Octadecenoic acid, methyl ester | *Terminalia catappa* | (Chikezie and Ekeanyanwu, 2020) | - |
|  | Diisooctyl phthalate | *Anacardium occidentale* | (Chikezie and Ekeanyanwu, 2020) | - |
|  | Trichloroacetic acid, hexadecyl ester Selenicereus undatus | *Selenicereus undatus* | (Luo et al., 2014) | - |
|  | Isopropyl linoleate | *Clerodendrum phlomidis* | (Jainab, 2017) | Antioxidant activity |
|  | Dodecane, 2,6,11-trimethyl-, | *Azanza garckeana* | (Luo et al., 2014) | - |
|  | Dodecyl acrylate | *Citrus macroptera* | (Rana and Blazquez, 2012) | - |
|  | Heptanoic acid, anhydride | *Phyllanthus amarus* | (Mamza et al., 2012) | - |
|  | 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester | *Syzygium aromaticum* | (Ingole, 2016; Muhammad et al., 2021; Rashmi et al., 2018) | Anti-bacterial |
|  | Isobutyl acetate | *Artabotrys hexapetalus.* | (Liu et al., 2020; Sowndhariya et al., 2022) | - |

References

1. Aneja, M., Gianfagna, T.J., Hebbar, P.K., 2005. Trichoderma harzianum produces nonanoic acid, an inhibitor of spore germination and mycelial growth of two cacao pathogens. Physiological and Molecular Plant Pathology 67, 304–307. https://doi.org/10.1016/j.pmpp.2006.05.002
2. Balachandran, P., Parthasarathy, V., Ajay Kumar, T.V., 2016. Isolation of Compounds from *Sargassum wightii*  by GCMS and the Molecular Docking against Anti-Inflammatory Marker COX2. ILCPA 63, 1–12. https://doi.org/10.56431/p-12582w
3. Balamurugan, V., Balakrishnan, V., Sundaresan, A., 2015. GC-MS analysis of leaf and Bark Extract of Moringa concanensis Nimmo, a siddha medicinal plant of South India. European Journal of Biotechnology and Bioscience 3, 57–61.
4. Bashari, M.H., Huda, F., Tartila, T.S., Shabrina, S., Putri, T., Qomarilla, N., Atmaja, H., Subhan, B., Sudji, I.R., Meiyanto, E., 2019. Bioactive Compounds in the Ethanol Extract of Marine Sponge Stylissa carteri Demonstrates Potential Anti-Cancer Activity in Breast Cancer Cells. Asian Pac J Cancer Prev 20, 1199–1206. https://doi.org/10.31557/APJCP.2019.20.4.1199
5. Chang, E.-H., Jung, S.-M., Hur, Y.-Y., 2014. Changes in the aromatic composition of grape cv. Cheongsoo wine depending on the degree of grape ripening. Food Science and Biotechnology 23, 1761–1771.
6. Chen, Y., Yin, H., Wu, X., Shi, X., Qi, K., Zhang, S., 2018. Comparative analysis of the volatile organic compounds in mature fruits of 12 Occidental pear (Pyrus communis L.) cultivars. Scientia Horticulturae 240, 239–248. https://doi.org/10.1016/j.scienta.2018.06.014
7. Chikezie, P.C., Ekeanyanwu, R.C., 2020. Phytocomponents from Anacardium occidentale, Psidium guajava, and Terminalia catappa altered membrane osmotic stability of sickle erythrocytes. Beni-Suef University Journal of Basic and Applied Sciences 9, 1–22.
8. Cueto, G.M., Zerba, E., Picollo, M.I., 2005. Biological effect of 1-dodecanol in teneral and post-teneral Rhodnius prolixus and Triatoma infestans (Hemiptera: Reduviidae). Mem Inst Oswaldo Cruz 100, 59–61. https://doi.org/10.1590/s0074-02762005000100012
9. Da Silva, M.L., Luz, A.I.R., Zoghbi, M.G.B., Ramos, L.S., Maia, J.G.S., 1984. Essential oils of some amazonian Mikania species. Phytochemistry 23, 2374–2376. https://doi.org/10.1016/S0031-9422(00)80558-0
10. Debi, C., Parkash, V., 2020. Influence of microbial bioinoculants on the accumulation of new phytocompounds in Oroxylum indicum (L.) Benth. ex Kurz. GSC Biological and Pharmaceutical Sciences 13, 228–243. https://doi.org/10.30574/gscbps.2020.13.3.0413
11. Deng, H., He, R., Long, M., Li, Y., Zheng, Y., Lin, L., Liang, D., Zhang, X., Liao, M., Lv, X., Deng, Q., Xia, H., 2021. Comparison of the Fruit Volatile Profiles of Five Muscadine Grape Cultivars (Vitis rotundifolia Michx.) Using HS-SPME-GC/MS Combined With Multivariate Statistical Analysis. Frontiers in Plant Science 12.
12. Ebin, T.U., 2021. Pharmaceutical study and Analysis of Gudoochi (Tinospora cordifolia Willd) Arka. International Journal of Ayurveda and Traditional Medicine 3, 11–15.
13. Gayathiri, E., Mahalakshmi, P., Pratheep, T., Prakash, P., Selvam, K., Manivasagaperumal, R., Ragunathan, M.G., Jayanthi, J., Kumaravel, P., 2022. In silico and in vitro approaches to evaluate the bioactivities of Chaetomorpha linum. South African Journal of Botany, Biotechnological exploration of natural products as functional food and medicine 151, 581–590. https://doi.org/10.1016/j.sajb.2022.06.067
14. Ge, S., Peng, W., Li, D., Mo, B., Zhang, M., Qin, D., 2015. Study on antibacterial molecular drugs in Eucalyptus granlla wood extractives by GC-MS. Pakistan journal of pharmaceutical sciences 28, 1445–1448.
15. Growther, L., Savitha, N., NirenAndrew, S., 2012. Antibacterial activity of punica granatum peel extracts against shiga toxin producing e. Coli.
16. Hadi Hameed, R., Mohammad, G., Hameed, I., 2018. Characterization of Antimicrobial Metabolites Produced by Salvadora persica and Analysis of Its Chemical Compounds Using GC-MS and FTIR. Indian Journal of Public Health Research and Development 9. https://doi.org/10.5958/0976-5506.2018.00216.4
17. Heidary Jamebozorgi, F., Yousefzadi, M., Firuzi, O., Nazemi, M., Jassbi, A.R., 2019. In vitro anti-proliferative activities of the sterols and fatty acids isolated from the Persian Gulf sponge; Axinella sinoxea. Daru 27, 121–135. https://doi.org/10.1007/s40199-019-00253-8
18. Ingole, S.N., 2016. Phytochemical analysis of leaf extract of Ocimum americanum L.(Lamiaceae) by GCMS method. World Scientific News 76–87.
19. Jainab, N.H., 2017. Antioxidant study of isolated chemical constituents from methanol extract of the Clerodendrum phlomidis leaf. World Journal of Pharmaceutical Research 6, 1122–1133.
20. Jayaraman, L., Shivaji, S., Anandakumar, S., 2022. Phytochemical screening, cytotoxic activity and molecular docking studies of Eclipta alba leaves extract against oral cancer. RJC 15, 676–685. https://doi.org/10.31788/RJC.2022.1516754
21. Joshi, R.K., 2011. GC/MS analysis of the essential oil of Senecio belgaumensis flowers. Nat Prod Commun 6, 1145–1146.
22. Kamatou, G.P.P., Viljoen, A.M., 2017. Comparison of fatty acid methyl esters of palm and palmist oils determined by GCxGC–ToF–MS and GC–MS/FID. South African Journal of Botany 112, 483–488. https://doi.org/10.1016/j.sajb.2017.06.032
23. Liu, C., Zhou, Q., Li, Y., Garner, L.V., Watkins, S.P., Carter, L.J., Smoot, J., Gregg, A.C., Daniels, A.D., Jervey, S., Albaiu, D., 2020. Research and Development on Therapeutic Agents and Vaccines for COVID-19 and Related Human Coronavirus Diseases. ACS Cent Sci 6, 315–331. https://doi.org/10.1021/acscentsci.0c00272
24. Luo, H., Cai, Y., Peng, Z., Liu, T., Yang, S., 2014. Chemical composition and in vitroevaluation of the cytotoxic and antioxidant activities of supercritical carbon dioxide extracts of pitaya (dragon fruit) peel. Chemistry Central Journal 8, 1–7.
25. Mamza, U.T., Sodipo, O., Khan, I.Z., 2012. Gas chromatography-mass spectrometry (gc-ms) analysis of bioactive components of phyllanthus amarus leaves.
26. Manilal, A., Sabu, K.R., Woldemariam, M., Aklilu, A., Biresaw, G., Yohanes, T., Seid, M., Merdekios, B., 2021. Antibacterial Activity of Rosmarinus officinalis against Multidrug-Resistant Clinical Isolates and Meat-Borne Pathogens. Evidence-Based Complementary and Alternative Medicine 2021, 1–10. https://doi.org/10.1155/2021/6677420
27. Muhammad, S.L., Wada, Y., Mohammed, M., Ibrahim, S., Musa, K.Y., Olonitola, O.S., Ahmad, M.H., Mustapha, S., Abdul Rahman, Z., Sha’aban, A., 2021. Bioassay-Guided Identification of Bioactive Compounds from Senna alata L. against Methicillin-Resistant Staphylococcus aureus. Applied Microbiology 1, 520–536. https://doi.org/10.3390/applmicrobiol1030034
28. Nirmal, C.R., Rajadas, S.E., Balasubramanian, M., Mohanvel, S.K., Aathi, M.S., Munishankar, S., Chilamakuru, N.B., Thiruvenkadam, K., Pandiya Raj, A.K., Paraman, R., Dusthackeer, A., 2022. Myoinositol and methyl stearate increases rifampicin susceptibility among drug-resistant Mycobacterium tuberculosis expressing Rv1819c. Chemical Biology & Drug Design n/a. https://doi.org/10.1111/cbdd.14197
29. Parthipan, B., Suky, M., Mohan, V., 2015. GC-MS analysis of phytocomponents in Pleiospermium alatum (Wall. ex Wight & Arn.) Swingle,(Rutaceae). Journal of Pharmacognosy and Phytochemistry 4, 216–222.
30. Payum, T., 2020. Phytoconstituents and proximate composition of clerodendrum colebrookianum walp.: a widely used anti high blood pressure medicinal food plant in eastern himalayas. Pharmacognosy Journal 12.
31. Rana, V.S., Blazquez, M.A., 2012. Compositions of the volatile oils of Citrus macroptera and C. maxima. Nat Prod Commun 7, 1371–1372.
32. Rangel-Sánchez, G., Castro-Mercado, E., García-Pineda, E., 2014. Avocado roots treated with salicylic acid produce phenol-2,4-bis (1,1-dimethylethyl), a compound with antifungal activity. J Plant Physiol 171, 189–198. https://doi.org/10.1016/j.jplph.2013.07.004
33. Rashmi, M., Meena, H., Meena, C., Kushveer, J.S., Busi, S., Murali, A., Sarma, V.V., 2018. Anti-quorum sensing and antibiofilm potential of Alternaria alternata, a foliar endophyte of Carica papaya, evidenced by QS assays and in-silico analysis. Fungal Biology 122, 998–1012. https://doi.org/10.1016/j.funbio.2018.07.003
34. Revathi, N., Dhanaraj, T.S., 2019. Evaluation of bioactive phytochemicals in leaves extract of Dodonaea angustifolia using gas chromatography and mass spectroscopic technique. J Pharmacogn Phytochem 8, 4406–4409.
35. Sahi, N., 2016. Evaluation of insecticidal activity of bioactive compounds from eucalyptus citriodora against tribolium castaneum 8, 1256–1270.
36. Sangeet, S., Khan, A., Mahanta, S., Roy, N., Das, S.K., Mohanta, Y.K., Saravanan, M., Tag, H., Hui, P.K., 2022. Computational analysis of Bacopa monnieri (L.) Wettst. compounds for drug development against Neurodegenerative Disorders. Curr Comput Aided Drug Des. https://doi.org/10.2174/1573409918666221010103652
37. Shah, B., Modi, P., Sagar, S.R., 2020. In silico studies on therapeutic agents for COVID-19: Drug repurposing approach. Life Sci 252, 117652. https://doi.org/10.1016/j.lfs.2020.117652
38. Shah, Z., Badshah, S., Iqbal, A., Emwas, A.-H., Jaremko, M., 2022. GC-MS based metabolomics and lipidiomics analyses of selected freshwater green macroalgae (preprint). In Review. https://doi.org/10.21203/rs.3.rs-1324666/v1
39. Sharma, A., Kumar, V., Singh, R., Thukral, A., Bhardwaj, R., 2015. 24-Epibrassinolide induces the synthesis of phytochemicals effected by imidacloprid pesticide stress in Brassica juncea L. J Pharmacogn Phytochem 4.
40. Siporin, C., Cooney, J.J., 1976. Inhibition of glucose metabolism by n-hexadecane in Cladosporium (Amorphotheca) resinae. J Bacteriol 128, 235–241.
41. Sonkar, P., 2019. Identification and Characterization of Antagonism Band of Secondary Metabolite from T. asperellum MK045610 against F. oxysporum f. sp. ciceri and F. oxysporum f. sp. lycopersici based on HPTLC and GC-MS. IJPE 5. https://doi.org/10.18811/ijpen.v5i03.11
42. Sowndhariya, S.S., Ravi, S., Dharani, J.D., Sripathi, R.S., 2022. Chemical Constitution, In-silico Molecular Docking Studies and Antibacterial Activity of Flower Essential Oil of Artabotrys hexapetalus. Jordan Journal of Pharmaceutical Sciences 15, 341–354. https://doi.org/10.35516/jjps.v15i3.408
43. Stroheker, T., Cabaton, N., Nourdin, G., Régnier, J.-F., Lhuguenot, J.-C., Chagnon, M.-C., 2005. Evaluation of anti-androgenic activity of di-(2-ethylhexyl)phthalate. Toxicology 208, 115–121. https://doi.org/10.1016/j.tox.2004.11.013
44. Xie, C., Wang, S., Cao, M., Xiong, W., Wu, L., 2022. (E)-9-Octadecenoic Acid Ethyl Ester Derived from Lotus Seedpod Ameliorates Inflammatory Responses by Regulating MAPKs and NF-*κ*B Signalling Pathways in LPS-Induced RAW264.7 Macrophages. Evidence-Based Complementary and Alternative Medicine 2022, e6731360. https://doi.org/10.1155/2022/6731360
45. Yao, X.T., Ling, P.X., Jiang, S., Lai, P.X., Zhu, C.G., 2013. Analysis of the essential oil from Gaillardia pulchella Foug. and its antioxidant activity. Journal of oleo science 62, 329–333.