**Table S 1.** Qualitative phytochemical analysis of bark and fruit extract of *B. retusa*.

|  |  |  |  |
| --- | --- | --- | --- |
| S. No. | Chemical Component | Methanol | Ethyl acetate |
| **Bark** | **Fruit** | **Bark** | **Fruit** |
|  | Alkaloids | **+** | **+** | **+** | **+** |
|  | Cardiac Glycosides | **+** | **+** | **+** | **+** |
|  | Flavonoids | **+** | **+** | **+** | **+** |
|  | Saponins | **+** | **+** | **-** | **-** |
|  | Steroids | **+** | **+** | **+** | **+** |
|  | Tannins | **+** | **+** | **-** | **-** |
|  | Terpenoids | **+** | **+** | **-** | **+** |
| The marks ‘+’ and ‘−’ indicate ‘present’ and ‘absent’, respectively. |

**Table S 2.** Biological activities of phytoconstituents of *B. retusa*.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| S. No. | Name of the compound | Compound nature | Biological activities | References |
|  | n-Hexadecanoic acid | fatty acid | antioxidant, anti-inflammatory, pesticide, nematicide activity | 54 |
|  | Furfural | aldehydes | food flavouring, pesticidal activity | 55 |
|  | Pyrovalerone | aromatic ketone | norepinephrine-dopamine reuptake inhibitor (NDRI), anorectic or appetite suppressant activity | 56 |
|  | Pyrogallol | phenol | antiseptic, cytotoxic, antioxidant, antibacterial, anti-inflammatory activity | 57 and 58 |
|  | Phytol | diterpene | anxiolytic, antimicrobial, antioxidant, antinociceptive, anti-inflammatory, cytotoxic, metabolism-modulating, apoptosis-inducing, immune-modulating activity | 59, 60 and 61 |
|  | Linoleic acid | fatty acid | essential for normal mammary tissue development | 62 |
|  | Erucylamide | fatty amide | regulate the central nervous system, antidepressant, and anti-anxiety, regulate hypothalamus-pituitary-adrenal axis (HPA), acetylcholinesterase inhibitory activity | 63 and 64 |
|  | Squalene | triterpene | provides skin protection, antistatic, antioxidant, anti-carcinogenic, vaccine adjuvants | 65 and 66 |
|  | Friedelin | pentacyclic triterpenoid | anti-inflammatory, analgesic, antipyretic, antioxidant, antimicrobial, vasodilator, anti-gastric ulcer, anti-diarrheal, liver protective, antidiabetic activity | 67 - 74 |
|  | *trans*-chrysanthenyl acetate | monoterpenoid | phytotoxic, antimicrobial, allelopathic, antifungal, antioxidant, tyrosinase inhibitory activity | 75 - 77 |
|  | Methyl octadeca-9,12-dienoate | \_ | antioxidant, anti-inflammatory, antibacterial, promotes the re-population of the seminiferous tubules with germ cells | 58, 78 and 79 |
|  | Methyl stearate | fatty acid ester | cytotoxic action on T-cell leukaemia cell line, cytotoxic to acute promyeloblastic leukaemia cell line, promotes migration ability of mesenchymal stem cells and accelerate cartilage regeneration, bio-herbicide, allelopathic, downregulate the essential parasitic nematode genes *Mi-flp-18* and *16D10* | 80 - 84 |
|  | Tridecane | alkane | antimicrobial activity, skin irritate | 85 and 86 |
|  | Dodecane, 2,6,11-trimethyl- | fatty acid | antibacterial, analgesic activity | 87 and 88 |
|  | Dodecane, 5,8-diethyl- | fatty acid | antibacterial activity | 89 |
|  | Hexane, 3,3-dimethyl- | alkane | insecticidal and repellent effects | 90 |
|  | Cetene | alkane | insecticidal activity | 91 |
|  | Methyl palmitate | fatty acid ester | bio-herbicide, reduction of plasma levels (TNF-α) & (IL-6), promote proliferation of mesenchymal stem cells, vasodilator effect of Nitric oxide, androgenic effect, cytoprotective potential, anti-inflammatory and antifibrotic effect, anti-arthritic effect, cardioprotective potential | 84 and 92 - 99 |
|  | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | lactone | antibacterial activity, anti-Alzheimer’s activity | 100 and 101 |
|  | Hexacosyl acetate | - | antioxidant activity | 102 |
|  | Tetratriacontane | ester | anticancer activity, antiviral activity against Influenza virus, anti-inflammatory activity | 103 - 105 |
|  | 3-Carene | monoterpene | inhibition activity against Main protease (Mpro) enzyme of Coronavirus 2, phyto-insecticides, antioxidant, neuroprotective, acaricide, larvicidal and anti-acetylcholinesterase, antifungal, antimicrobial activity | 106 - 111 |
|  | Sylvestrene | monoterpenoid | antimicrobial, antioxidant, anti- Alzheimer's, effective against diabetes mellitus, larvicidal activity | 112 - 115 |
|  | 1-Hexanol, 2-ethyl- | fatty alcohol | growth inhibition, autophagy, apoptosis induction activity | 116 |
|  | Imidazole | azole | anti-tubercular activity, antibacterial, antiviral, antioxidant, anti-inflammatory, antidiabetic, antimycobacterial, antifungal, antitumor, anti-allergic, anti-amoebic, antipyretic, antihelmintic and ulcerogenic activities, effective against Alzheimer's disease, modulate gene expression activity | 117 - 120 |
|  | 2,4-Imidazolidinedione, 3-methyl- | - | antifungal and antibacterial activity | 121 |
|  | Dodecane, 2,6,11-trimethyl- | alkane | antibacterial potential, analgesic properties | 87 - 88 |
|  | Tromethamine | primary amino compound | used as COVID-19 vaccine components | 122 and 123 |
|  | 1-Undecanol | fatty alcohol | fungicide activity | 124 |
|  | 10-Methylnonadecane | - | mutagenic activity | 125 |
|  | Trichloroacetic acid, hexadecyl ester | organo-halogen compound | cytotoxic and antioxidant activity | 126 |
|  | 2-Isopropyl-5-methyl-1-heptanol | alcohol | antifungal activity | 127 |
|  | 1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester | phthalic acid | reprotoxic and endocrine disruptor used in medical devices | 128 and 129 |
|  | Diisooctyl phthalate | phthalic acid | anti-quorum sensing potential and prevented the biofilm synthesis, inhibits the activity (elastase and protease) and virulence factors, antibacterial activity; inhibit G protein-coupled cannabinoid-1 (CB1) receptor activity | 130 -132 |

**Table S 3.** Bioactive compounds, organic substances, or volatile compounds identified in the methanol fruit extract of *B. retusa* using gas chromatography-mass spectrometry, *CAS* chemical abstract service.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S. No. | CAS | Name of the compound | Molecular Formula | Molecular weight | Peak area (%) |
|  | 98-01-1 | Furfural | C5H4O2 | 96 | 2.136% |
|  | 56-81-5 | Glycerin | C3H8O3 | 92 | 3.311% |
|  | 3563-49-3 | Pyrovalerone | C16H23NO | 245 | 2.833% |
|  | 28564-83-2 | Pyranone | C6H8O4 | 144 | 1.832% |
|  | 67-47-0 | Hydroxymethylfurfural | C6H6O3 | 126 | 20.708% |
|  | 123232-57-5 | 3-Octanol, 2,6-dimethyl-, acetate | C12H24O2 | 200 | 3.058% |
|  | 53907-91-8 | 1,4-Dioxane, 2-ethyl-5-methyl- | C7H14O2 | 130 | 0.907% |
|  | 87-66-1 | Pyrogallol | C6H6O3 | 126 | 4.713% |
|  | 2595-97-3 | D-Allose | C6H12O6 | 180 | 10.052% |
|  | 3396-99-4 | α-D-Galactopyranoside, methyl | C7H14O6 | 194 | 0.954% |
|  | 3458-28-4 | d-Mannose | C6H12O6 | 180 | 3.015% |
|  | 544-63-8 | Tetradecanoic acid | C14H28O2 | 228 | 1.013% |
|  |  | 3-O-Methyl-d-glucose | C7H14O6 | 194 | 5.356% |
|  | 112-39-0 | Hexadecanoic acid, methyl ester | C17H34O2 | 270 | 0.528% |
|  | 6386-38-5 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester | C18H28O3 | 292 | 2.006% |
|  | 57-10-3 | n-Hexadecanoic acid or Palmitic acid | C16H32O2 | 256 | 8.254% |
|  | 142-91-6 | Isopropyl palmitate | C19H38O2 | 298 | 0.118% |
|  |  | Heptanoic acid, 4-octyl ester | C15H30O2 | 242 | 0.361% |
|  | 2462-85-3 | 9,12-Octadecadienoic acid, methyl ester | C19H34O2 | 294 | 0.755% |
|  | 2777-58-4 | Methyl petroselinate | C19H36O2 | 296 | 1.433% |
|  | 150-86-7 | Phytol | C20H40O | 296 | 0.190% |
|  | 5129-61-3 | Heptadecanoic acid, 16-methyl-, methyl ester | C19H38O2 | 298 | 0.244% |
|  | 60-33-3 | Linoleic acid | C18H32O2 | 280 | 19.652% |
|  | 57-11-4 | Octadecanoic acid | C18H36O2 | 284 | 4.162% |
|  | 506-30-9 | Eicosanoic acid (Arachidic acid) | C20H40O2 | 312 | 0.100% |
|  | 59130-69-7 | Hexanoic acid, 2-ethyl-, hexadecyl ester | C24H48O2 | 368 | 0.368% |
|  | 29899-13-6 | Hexadecanoic acid, 2-(octadecyloxy)ethyl ester | C36H72O3 | 552 | 0.037% |
|  | 23470-00-0 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | C19H38O4 | 330 | 0.087% |
|  | 131-20-4 | Diisooctyl phthalate | C24H38O4 | 390 | 0.086% |
|  | 59130-70-0 | Hexanoic acid, 2-ethyl-, octadecyl ester | C26H52O2 | 396 | 0.145% |
|  | 112-84-5 | Erucylamide | C22H43NO | 337 | 0.260% |
|  | 111-02-4 | Squalene | C30H50 | 410 | 0.123% |
|  | 105-92-0 | Rhodopin | C40H58O | 554 | 0.498% |
|  | 559-74-0 | Friedelin | C30H50O | 426 | 0.707% |

**Table S 4.** Bioactive compounds, organic substances, or volatile compounds identified in the methanol bark extract of *B. retusa* using gas chromatography-mass spectrometry, *CAS* chemical abstract service.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S. No. | CAS | Name of the compound | Molecular Formula | Molecular weight | Peak area (%) |
|  | 141-78-6 | Ethyl Acetate | C4H8O2 | 88 | 0.367% |
|  | 109-60-4 | Propyl acetate | C5H10O2 | 102 | 0.054% |
|  | 50764-55-1 | trans-Chrysanthenyl acetate | C12H18O2 | 194 | 0.019% |
|  | 112-42-5 | 1-Undecanol | C11H24O | 172 | 0.020% |
|  | 5129-65-7 | Dodecanoic acid, 10-methyl-, methyl ester | C14H28O2 | 228 | 0.086% |
|  | 6422-86-2 | Dioctyl terephthalate | C24H38O4 | 390 | 0.228% |
|  | 2156-97-0 | Dodecyl acrylate | C15H28O2 | 240 | 2.388% |
|  |  | Terephthalic acid, 4-octyl octyl ester | C24H38O4 | 390 | 10.368% |
|  | 2462-85-3 | Methyl octadeca-9,12-dienoate | C19H34O2 | 294 | 0.135% |
|  |  | trans-13-Octadecenoic acid, methyl ester | C19H36O2 | 296 | 0.330% |
|  | 112-61-8 | Methyl stearate | C19H38O2 | 298 | 0.101% |
|  | 103-23-1 | Hexanedioic acid, bis(2-ethylhexyl) ester | C22H42O4 | 370 | 2.279% |

**Table S 5.** Bioactive compounds, organic substances, or volatile compounds identified in the ethyl acetate fruit extract of *B. retusa* using gas chromatography-mass spectrometry, *CAS* chemical abstract service.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S. No. | CAS | Name of the compound | Molecular Formula | Molecular weight | Peak area (%) |
|  | 629-50-5 | Tridecane | C13H28 | 184 | 0.806% |
|  | 62016-18-6 | Octane, 5-ethyl-2-methyl- | C11H24 | 156 | 0.564% |
|  | 7206-26-0 | 2-Dodecene, (Z)- | C12H24 | 168 | 0.654% |
|  | 31295-56-4 | Dodecane, 2,6,11-trimethyl- | C15H32 | 212 | 0.478% |
|  | 629-62-9 | Pentadecane | C15H32 | 212 | 0.036% |
|  | 24251-86-3 | Dodecane, 5,8-diethyl- | C16H34 | 236 | 0.033% |
|  | 17301-32-5 | Undecane, 4,7-dimethyl- | C13H28 | 184 | 0.238% |
|  | 563-16-6 | Hexane, 3,3-dimethyl- | C8H18 | 114 | 0.059% |
|  | 629-73-2 | Cetene | C16H32 | 224 | 1.836% |
|  | 544-76-3 | Hexadecane | C16H34 | 226 | 0.804% |
|  | 504-44-9 | Hexadecane, 2,6,11,15-tetramethyl- | C20H42 | 282 | 0.843% |
|  | 27458-90-8 | Disulfide, di-tert-dodecyl | C24H50S2 | 402 | 0.150% |
|  | 54833-48-6 | Heptadecane, 2,6,10,15-tetramethyl- | C21H44 | 296 | 0.235% |
|  | 1560-84-5 | Eicosane, 2-methyl- | C21H44 | 296 | 0.440% |
|  | 5333-42-6 | Eutanol G | C20H42O | 298 | 0.298% |
|  | 6418-44-6 | Heptadecane, 3-methyl- | C18H38 | 254 | 0.201% |
|  | 2136-72-3 | 2-Octadecoxyethanol | C20H42O2 | 314 | 0.043% |
|  | 2420-38-4 | Octadecanoic acid, 4-hydroxy-, methyl ester | C19H38O3 | 314 | 0.200% |
|  | 64437-47-4 | Hexadecen-1-ol, trans-9- | C16H32O | 240 | 1.082% |
|  | 150-86-7 | Phytol | C20H40O | 296 | 0.293% |
|  | 10152-66-6 | Cyclopropaneoctanoic acid, 2-[(2-pentylcyclopropyl)methyl]-, methyl ester, trans,trans- | C21H38O2 | 322 | 0.499% |
|  | 112-39-0 | Hexadecanoic acid, methyl ester or Methyl palmitate | C17H34O2 | 270 | 0.458% |
|  | 82304-66-3 | 7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione | C17H24O3 | 276 | 0.371% |
|  | 6386-38-5 | Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester | C18H28O3 | 292 | 0.334% |
|  | 55333-99-8 | Eicosane, 7-hexyl- | C26H54 | 366 | 0.384% |
|  | 57-10-3 | n-Hexadecanoic acid or Palmitic acid | C16H32O2 | 256 | 21.824% |
|  | 14852-31-4 | 2-Hexadecanol | C16H34O | 242 | 2.091% |
|  | 626-27-7 | Heptanoic acid, anhydride | C14H26O3 | 242 | 0.687% |
|  | 56599-58-7 | 8,11-Octadecadienoic acid, methyl ester | C19H34O2 | 294 | 0.803% |
|  | 13481-95-3 | 10-Octadecenoic acid, methyl ester | C19H36O2 | 296 | 1.259% |
|  | 112-61-8 | Methyl stearate | C19H38O2 | 298 | 0.148% |
|  | 55282-12-7 | Octadecane, 3-ethyl-5-(2-ethylbutyl)- | C26H54 | 366 | 0.213% |
|  | 60-33-3 | Linoleic acid | C18H32O2 | 280 | 39.768% |
|  | 57-11-4 | Octadecanoic acid | C18H36O2 | 284 | 10.517% |
|  | 95008-11-0 | 10-Heneicosene (c,t) | C21H42 | 294 | 0.564% |
|  | 822-32-2 | Hexacosyl acetate | C28H56O2 | 424 | 0.212% |
|  | 59130-69-7 | Hexanoic acid, 2-ethyl-, hexadecyl ester | C24H48O2 | 368 | 0.369% |
|  | 14167-59-0 | Tetratriacontane | C34H70 | 478 | 4.728% |

**Table S 6.** Bioactive compounds, organic substances, or volatile compounds identified in the ethyl acetate bark extract of *B. retusa* using gas chromatography-mass spectrometry, *CAS* chemical abstract service.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| S. No. | CAS | Name of the compound | Molecular Formula | Molecular weight | Peak area (%) |
|  | 110-19-0 | Isobutyl acetate | C6H12O2 | 116 | 0.358% |
|  | 13466-78-9 | 3-Carene | C10H16 | 136 | 0.169% |
|  | 1461-27-4 | Sylvestrene | C10H16 | 136 | 0.325% |
|  | 104-76-7 | 1-Hexanol, 2-ethyl- | C8H18O | 130 | 0.257% |
|  | 288-32-4 | Imidazole | C3H4N2 | 68 | 0.392% |
|  | 56-81-5 | Glycerin | C3H8O3 | 92 | 0.811% |
|  | 6843-45-4 | 2,4-Imidazolidinedione, 3-methyl- | C4H6N2O2 | 114 | 0.396% |
|  | 31295-56-4 | Dodecane, 2,6,11-trimethyl- | C15H32 | 212 | 0.237% |
|  | 77-86-1 | Tromethamine | C4H11NO3 | 121 | 0.957% |
|  | 112-42-5 | 1-Undecanol | C11H24O | 172 | 0.881% |
|  | 56862-62-5 | 10-Methylnonadecane | C20H42 | 282 | 0.190% |
|  | 504-44-9 | Crocetane | C20H42 | 282 | 0.256% |
|  |  | 3-Chloropropionic acid, heptadecyl ester | C20H39ClO2 | 346 | 10.192% |
|  | 5333-42-6 | Eutanol G | C20H42O | 298 | 0.285% |
|  | 110225-00-8 | 1-Dodecanol, 2-hexyl- | C18H38O | 270 | 0.224% |
|  | 74339-54-1 | Trichloroacetic acid, hexadecyl ester | C18H33Cl3O2 | 386 | 0.340% |
|  | 91337-07-4 | 2-Isopropyl-5-methyl-1-heptanol | C11H24O | 172 | 0.437% |
|  | 6422-86-2 | 1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester | C24H38O4 | 390 | 5.791% |
|  |  | Terephthalic acid, 4-octyl octyl ester | C24H38O4 | 390 | 3.565% |
|  |  | Terephthalic acid, 3-hexyl octyl ester | C22H34O4 | 362 | 8.600% |
|  | 2136-72-3 | Ethanol, 2-(octadecyloxy)- | C20H42O2 | 314 | 0.203% |
|  | 109-43-3 | Decanedioic acid, dibutyl ester | C18H34O4 | 314 | 0.378% |
|  |  | 2-Methyl-Z-4-tetradecene | C15H30 | 210 | 0.347% |
|  |  | Heptacosyl pentafluoropropionate | C30H55F5O2 | 542 | 0.362% |
|  | 103-23-1 | Hexanedioic acid, bis(2-ethylhexyl) ester | C22H42O4 | 370 | 0.288% |
|  | 59130-69-7 | Hexanoic acid, 2-ethyl-, hexadecyl ester | C24H48O2 | 368 | 0.550% |
|  | 131-20-4 | Diisooctyl phthalate | C24H38O4 | 390 | 0.406% |
|  | 55333-99-8 | Eicosane, 7-hexyl- | C26H54 | 366 | 0.454% |
|  | 59130-70-0 | Hexanoic acid, 2-ethyl-, octadecyl ester | C26H52O2 | 396 | 0.605% |