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# GC-MS Analysis and Molecular Docking Studies of *Lavandula dentata* Leaves Extract of Taif Region, Saudi Arabia

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## ABSTRACT

**Background:** *Lavandula dentata* is recognized for its therapeutic properties and has been traditionally used in various medicinal applications. Monoamine oxidases (MAOs) are critical for neurotransmitters breaking down; therefore, their inhibitors treat neurodegenerative disorders such as Alzheimer, Parkinson and amyotrophic lateral sclerosis diseases.

**Methods:** The current study was done to analyze the bioactive compounds present in the methanolic extract of *Lavandula dentata* of Taif region, Saudi Arabia using Gas Chromatography-Mass Spectrometry (GC-MS) analysis. In addition, computational analysis using SwissADME and ProTox-II was used to predict the physicochemical and biological activities and predicted toxicity of four selected components from lavender extract. Moreover, linalool and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid were selected for the molecular docking of Monoamine Oxidase A.

**Result:** GC-MS analysis revealed a diverse array of bioactive compounds, including but not limited to linalool, retinal, chromene-2-one and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid, which are known for their pharmacological activities such as antimicrobial, anti-inflammatory and anxiolytic effects. *In silico* analysis has assumed that linalool is safe with a predicted toxicity LD50 2200 mg/kg (Class: 5). The docking affinity score of linalool to Monoamine Oxidase A is -24.4 and appears more stable in the docking site box due to the presence of nine hydrophobic interactions. Collectively this study contributes to the understanding of the chemical profile of *Lavandula dentata* and highlights its suitability for pharmaceutical and therapeutic applications along with exploring the specific bioactivities and potential synergistic effects of these compounds. In particular, linalool emerges as a promising bioactive compound in neurodegenerative disorders therapy through Monoamine oxidase A inhibition.


**Key words:** GC-MS analysis, *In silico*, *Lavandula dentata*, Linalool, Monoamine oxidase A, Taif.

## INTRODUCTION

*Lavandula* spp. is one of the most cultivated plants worldwide due to its essential oil properties. Several studies have demonstrated its antimicrobial and biological activities (Carrasco *et al*., 2016; de Rapper *et al*., 2016). This genus consists of 39 species, along with approximately 400 registered cultivars and several hybrids (Benabdelkader *et al*., 2011). The major compounds of *Lavandula* and its essential oil are linalool, linalyl acetate and alpha-terpineol (Speranza *et al*., 2023). However, the chemical composition of essential oils from the same plant species varies qualitatively and quantitatively depending on environmental conditions and their processing method (Asekun *et al*., 2007; Singh *et al*., 2008). *Lavandula dentata* L., belonging to the family *Lamiaceae*, is a widespread wild herb that grows in Saudi Arabia as well as in many other countries worldwide (Al-Sarar *et al*., 2014).

*Lavandula dentata* L. is a medicinal plant commonly used in traditional medicine to treat different diseases (Bouyahya *et al*., 2023). It was reported that *L. dentata* extracts and essential oils can be used as an antioxidant, anticancer, antiparasitic, antidiarrheal, antispasmodic, antihypertensive, antibacterial, antilithiasic, antifungal, anti-inflammatory and in treatment of neurological, gastrointestinal, urinary, genital, musculoskeletal and dermatological diseases (Belhaj *et al*., 2021; Djaballah and Bellaka, 2020; Fouad and Lahcen, 2020; Imen *et al*., 2021; Justus *et al*., 2019a, 2019b; Mohammed *et al*., 2020; Mrabti *et al*., 2019). These biological activities of *L. dentata* could be assigned to their bioactive compounds of flavonoids, tannins, terpenoids and anthracene derivatives (Imen *et al*., 2021).

Spectrometric and chromatographic methods to screen medicinal plants provide fundamental information on their chemical and pharmacological activities. This information is crucial in identifying plants with biological activity (Juszczak *et al*., 2019). Recently, gas chromatography-mass spectrometry (GC-MS) and Fourier-transform infrared (FTIR) have commonly been used for functional groups detection and identification of different bioactive therapeutic

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compounds that are present in medicinal plants (Fan *et al*., 2018; Satapute *et al*., 2019). However, GC-MS analysis represents one of the best, fastest and most accurate techniques for various compounds detection such as alkaloids, nitro compounds, alcohols, long-chain hydrocarbons, steroids, esters, organic acids and amino acids (Razack *et al*., 2015).

Monoamine oxidases (MAOs) are mitochondrial enzymes with two isotypes A and B. Their function is the breakdown of monoamine neurotransmitters including dopamine, adrenaline, serotonin, noradrenaline, β-phenylethylamine, norepinephrine and tyramine. MAO-A has a greater affinity for serotonin and noradrenaline as hydroxylated amines. MAOs overexpression can lead to mitochondrial damage that in turn could lead to a neurotoxic nature, depression, Alzheimer's disease and Parkinson's disease. Blocking MAOs with small molecules has advanced treatment for neuropsychiatric disorders and neurodegenerative diseases. Many MAO inhibitors have been developed since the 1960s, however, MAO inhibitors usage is linked to health improvement, mental/neurological diseases, off-target effects, safety concerns, dietary restrictions and low tyramine intake (Aljanabi *et al*., 2021; Kumar *et al*., 2024; Özdemir *et al*., 2021).

In the present study, we used the GC-MS technique to detect and identify the phytochemical compounds present in lavender leaves methanolic extract that is cultivated in the Taif region of Saudi Arabia. In Silico computational analysis was done using SwissADME and ProTox-II to predict the physicochemical, biological activities and predicted toxicity (lethal dose, LD50) of four select components from the extract of *Lavadula* methanolic extract. In addition, molecular docking was done using linalool and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid to Monoamine Oxidase A enzyme.

## MATERIALS AND METHODS

The experiment was conducted at Taif University in the summer season of 2023. *Lavandula dentata* L. were freshly collected from Taif region, Saudi Arabia (21°16′30.34″N 40°24′22.16″E). Before use, leaves were rinsed in water, dried away from the sun, collected and ground in an electric grinder to obtain fine powder. The powder was mixed with methanol (200 mL), macerated overnight and then filtered. The marc was macerated in methanol for 1 h and then filtered, this step was repeated twice. Finally, we obtained 600 ml of the collected methanol that was evaporated under vacuum at 40°C to yield 1.289 g of lavender leaves methanolic extract (LE) (Labarbe *et al*., 1999).

Gas chromatography-mass spectroscopy (GC-MS) is an ideal technique for phytoconstituents characterization to predict their structure, name, formula and retention time. RTX-5 MS capillary column (Restek) was used to chemically characterize the 95% methanolic LE with the help of GC-MS-QP2010 Plus system (Shimadzu, Japan) (Siddiqui *et al*., 2015). GC separates the various constituents into their components with their variable retention times and a mass spectrophotometer identifies the components. A chromatogram of relative abundance against retention time was produced by the software, coupled to the mass spectrophotometer.

We have selected the most abundant compounds from the extract to be used further in molecular docking analysis. The 3D conformations of selected compounds (ligands) were downloaded from the PubChem database. The 3D crystal structure of human Amine Oxidase A (receptor protein) with Harmine (actual co-crystallized ligand) (PDB ID: 2z5x with resolution 2.20 Å) was retrieved from RCSB PDB (http://www.rcsb.org/pdb/home/home.do). All water molecules, cofactor (FAD) and ligand (Harmine) were removed from the receptor protein by using PyMOL software.

The free online service SwissADME was used to predict their physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry (http://www. swissadme.ch/) (Daina *et al*., 2014; 2017; Daina and Zoete, 2016). The best-docked compounds were selected according to Lipinski's rule of five. Compounds that obey the Lipinski rule are considered ideal drug candidates. Lipinski stated that a compound could display drug-like behaviour if it does not fail more than one of the criteria: molecular weight not more than 500; hydrogen bond donors ≤5 and acceptors ≤10; lipophilicity less than 5 and molar refractivity between 40 and 130 (Lipinski *et al*., 2012).

Predicted toxicities and the Lethal Dose (LD50) predictions of the studied compounds were obtained using a ProTox-II web server (https://tox-new.charite.de/protox_II/) (Banerjee *et al*., 2018). SMINA/Anaconda was used in the molecular docking of selected compounds into the binding pockets of the receptor protein. The re-docking procedure was also applied to validate the accuracy of the docking protocol (Boström *et al*., 2003). Docking validation was done by redocking the co-crystallized ligand (Harmine) to the active site by using the ad4_scoring function. The best-docked conformations have been chosen by comparing the root mean squared deviation (RMSD) values with the actual co-crystallized ligand against the protein (Hevener *et al*., 2009). After docking, all the complex images were analyzed by using the Protein Ligand Interaction Profiler (PLIP, https://plip-tool.biotec.tu-dresden.de/plip-web/plip/index) to identify non-covalent interactions between protein and their ligands and their 2D images (Adasme *et al*., 2021).

## RESULTS AND DISCUSSION

Gas Chromatography-Mass Spectrometry (GC-MS) analysis has become a pivotal technique in the identification and characterization of bioactive compounds in various botanical extracts (Adams, 2007). In the current study, *Lavandula dentata* leaves methanolic extract underwent GC-MS analysis to elucidate its chemical composition.

The GC-MS analysis revealed a complex mixture of more than one hundred compounds with different retention time within the methanolic extract of *Lavandula dentata* leaves as displayed in Fig 1 and Table 1-3. One of the

**Table 1: GC-MS identified compounds in the methanolic extract of *Lavandula dentate***

| RT | Compound Name | Area % | MF | Molecular Formula | Molecular Weight | Cas # | Library |
|---|---|---|---|---|---|---|---|
| 7.75 | Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester | 1.40 | 723 | C26H50O2 | 394 | 52355-4 2-7 | mainlib |
| 7.75 | CYCLOPROPANETETRADECAN OIC ACID, 2-OCTYL-, METHYL ESTER | 1.40 | 722 | C26H50O2 | 394 | 52355-4 2-7 | WileyRegi stry8e |
| 7.75 | l-Gala-l-ido-octose | 1.40 | 721 | C8H16O8 | 240 | NA | mainlib |
| 7.75 | Oleic Acid | 1.40 | 689 | C18H34O2 | 282 | 112-80 -1 | replib |
| 7.75 | 9-OCTADECENOIC ACID | 1.40 | 689 | C18H34O2 | 282 | NA | WileyRegi stry8e |
| 12.75 | 1,6-Pentalenedione, hexahydro-6a-(2-propynyl)-, cis- | 1.58 | 716 | C11H12O2 | 176 | 92485-8 7-5 | mainlib |
| 12.75 | 1,6-PENTALENEDIONE, HEXAHYDRO-6A-(2-PROPYNYL) -, CIS- | 1.58 | 716 | C11H12O2 | 176 | 92485-8 7-5 | WileyRegi stry8e |
| 12.75 | (5-Oxo-1,3a,4,5,6,6a-hexahydropenta len-1-yl)-acetaldehyde | 1.58 | 695 | C10H12O2 | 164 | NA | mainlib |
| 12.75 | (5-OXO-1,3A,4,5,6,6A-HEXAHYD RO-1-PENTALENYL)ACETALDE HYDE | 1.58 | 695 | C10H12O2 | 164 | NA | WileyRegi stry8e |
| 12.75 | Tetracyclo[3.3.1.0.1(3,9)]decan-10-o ne | 1.58 | 724 | C10H12O | 148 | 16492-0 6-1 | mainlib |
| 12.86 | 1,6 Pentalenedione, hexahydro-6a-(2-propynyl)-, cis- | 0.46 | 714 | C11H12O2 | 176 | 92485 8 7-5 | mainlib |
| 12.86 | 1,6-PENTALENEDIONE, HEXAHYDRO-6A-(2-PROPYNYL) -, CIS- | 0.46 | 714 | C11H12O2 | 176 | 92485-8 7-5 | WileyRegi stry8e |
| 12.86 | Tetracyclo[3.3.1.0.1(3,9)]decan-10-o ne | 0.46 | 716 | C10H12O | 148 | 16492-0 6-1 | mainlib |
| 12.86 | TETRACYCLO[3.3.1.0.1(3,9)]DECA N-10-ONE | 0.46 | 716 | C10H12O | 148 | 16492-0 6-1 | WileyRegi stry8e |
| 12.86 | (6-Hydroxymethyl-2,3-dimethylphen yl)methanol | 0.46 | 700 | C10H14O2 | 166 | NA | mainlib |
| 14.11 | 2H-1-BENZOPYRAN-2-ONE | 10.64 | 926 | C9H6O2 | 146 | 91-64-5 | WileyRegi stry8e |
| 14.11 | 2H-1-BENZOPYRAN-2-ONE | 10.64 | 924 | C9H6O2 | 146 | 91-64-5 | WileyRegi stry8e |
| 14.11 | CHROMEN-2-ONE | 10.64 | 884 | C9H6O2 | 146 | NA | WileyRegi stry8e |
| 14.11 | CHROMEN-2-ONE | 10.64 | 882 | C9H6O2 | 146 | 91-64-5 | WileyRegi stry8e |
| 14.11 | 2H-1-BENZOPYRAN-2-ONE | 10.64 | 907 | C9H6O2 | 146 | 91-64-5 | WileyRegi stry8e |
| 18.85 | Cyclopenta[1.3]cyclopropa[1.2]cyclo hepten-3(3aH)-one, 1,2,3b,6,7,8-hexahydro-6,6-dimethyl- | 1.03 | 755 | C13H18O | 190 | 91531-5 8-7 | mainlib |
| 18.85 | CYCLOPENTA[1,3]CYCLOPROP A[1,2]CYCLOHEPTEN 3(3AH) ON E, 1,2,3B,6,7,8-HEXAHYDRO-6,6-DI METHYL- | 1.03 | 755 | C13H18O | 190 | 91531-5 8 7 | WileyRegi stry8e |
| 18.85 | 8-Isopropenyl-1,3,3,7-tetramethyl-bi cyclo[5.1.0]oct-5-en-2-one | 1.03 | 744 | C15H22O | 218 | NA | mainlib |
| 18.85 | 8-ISOPROPENYL-1,3,3,7-TETRAM ETHYL-BICYCLO[5.1.0]OCT-5-E N-2-ONE | 1.03 | 744 | C15H22O | 218 | NA | WileyRegi stry8e |
| 18.85 | Cedran-diol, 8S,13- | 1.03 | 732 | C15H26O2 | 238 | 88588-4 8-1 | mainlib |
| 18.99 | Retinal | 0.84 | 802 | C20H28O | 284 | 116-31 -4 | mainlib |
| 18.99 | RETINAL | 0.84 | 802 | C20H28O | 284 | 116-31 -4 | WileyRegi stry8e |
| 18.99 | Ppropiolic acid, 3-(1-hydroxy-2-isopropyl-5-methylcy clohexyl)- | 0.84 | 741 | C13H20O3 | 224 | NA | mainlib |
| 18.99 | 3-(1-HYDROXY-2-ISOPROPYL-5-M ETHYLCYCLOHEXYL)-2-PROPY NOIC ACID | 0.84 | 741 | C13H20O3 | 224 | NA | WileyRegi stry8e |
| 18.99 | Spiro[4.5]dec-6-en-8-one, 1,7-dimethyl-4-(1-methylethyl)- | 0.84 | 719 | C15H24O | 220 | 39510-3 6-6 | mainlib |
| 19.64 | 2-Naphthalenemethanol, decahydro-à,à,4a-trimethyl-8-methyle ne-, [2R-(2à,4aà,8aà)]- | 1.67 | 878 | C15H26O | 222 | 473-15 -4 | replib |
| 19.64 | 2-NAPHTHALENEMETHANOL, DECAHYDRO-à,à,4A,8-TETRAM ETHYL-, DIDEHYDRO DERIV., [2R-(2à,4Aà,8Aà)]- | 1.67 | 802 | C15H26O | 222 | 51317-0 8-9 | WileyRegi stry8e |
| 19.64 | 2-NAPHTHALENEMETHANOL, DECAHYDRO-à,à,4A-TRIMETHY L-8-METHYLENE-, [2R-(2à,4Aà,8Aà)]- | 1.67 | 802 | C15H26O | 222 | 473-15 -4 | WileyRegi stry8e |
| 19.64 | 2-NAPHTHALENEMETHANOL, DECAHYDRO-à,à,4A-TRIMETHY L-8-METHYLENE-, [2R-(2à,4Aà,8Aà)]- | 1.67 | 867 | C15H26O | 222 | 473-15 -4 | WileyRegi stry8e |
| 19.64 | 2-Naphthalenemethanol, decahydro-à,à,4a-trimethyl-8-methyle ne-, [2R-(2à,4aà,8aà)]- | 1.67 | 810 | C15H26O | 222 | 473-15 -4 | mainlib |
| 20.16 | 2-CYCLOHEXEN-1-ONE, 2,4,4-TRIMETHYL-3-(3-OXO-1-B UTENYL)- | 1.20 | 821 | C13H18O2 | 206 | 27185-7 7-9 | WileyRegi stry8e |
| 20.16 | 4-(2-ACETYL-5,5-DIMETHYL-2-CY CLOPENTEN-1-YLIDENE)-2-BUTA NONE | 1.20 | 742 | C13H18O2 | 206 | NA | WileyRegi stry8e |
| 20.16 | 4-(2-ACETYL-5,5-DIMETHYL-2-CY CLOPENTEN-1-YLIDENE)-2-BUTA NONE | 1.20 | 742 | C13H18O2 | 206 | NA | WileyRegi stry8e |
| 20.16 | 4-(2-Acetyl-5,5-dimethylcyclopent-2 -enylidene)butan-2-one | 1.20 | 740 | C13H18O2 | 206 | NA | mainlib |
| 20.16 | ETHYL 3-(1-HYDROXY-2-ISOPROPYL-5-M ETHYLCYCLOHEXYL)-2-PROPYN | 1.20 | 732 | C15H24O3 | 252 | NA | WileyRegi stry8e |
| 20.79 | 1-Methyl-1-(o-methylphenyl)-1-silacy clobutane | 1.37 | 707 | C11H16Si | 176 | NA | mainlib |
| 20.79 | 1,6-Pentalenedione, hexahydro-6a-(2-propynyl)-, cis- | 1.37 | 694 | C11H12O2 | 176 | 92485-8 7-5 | mainlib |
| 20.79 | 1,6-PENTALENEDIONE, HEXAHYDRO-6A-(2-PROPYNYL) -, CIS- | 1.37 | 694 | C11H12O2 | 176 | 92485-8 7-5 | WileyRegi stry8e |
| 20.79 | 1-HEXENE, 2-(O-ANISYL)-4-METHYL- | 1.37 | 694 | C14H20O | 204 | NA | WileyRegi stry8e |
| 20.79 | 2H-1-Benzopyran-2-one, 7-methoxy- | 1.37 | 881 | C10H8O3 | 176 | 531-59 -9 | replib |
| 20.86 | 1-Methyl-1-(o-methylphenyl)-1-silacy clobutane | 0.47 | 791 | C11H16Si | 176 | NA | mainlib |
| 20.86 | 2H-1-Benzopyran-2-one, 8-methoxy- | 0.47 | 740 | C10H8O3 | 176 | 2445-8 1-0 | mainlib |
| 20.86 | 2H-1-BENZOPYRAN-2-ONE, 8-METHOXY- | 0.47 | 740 | C10H8O3 | 176 | 2445-8 1-0 | WileyRegi stry8e |
| 20.86 | Cumarin-3-carboxylic acid, 7-methoxy- | 0.47 | 713 | C11H8O5 | 220 | 20300-5 9-8 | mainlib |

**Table 2: GC-MS identified compounds in the methanolic extract of *Lavandula dentate***

| RT | Compound Name | Area % | MF | Molecular Formula | Molecular Weight | Cas # | Library |
|---|---|---|---|---|---|---|---|
| 20.98 | 2H-1-Benzopyran-2-one, 8-methoxy- | 0.77 | 738 | C10H8O3 | 176 | 2445-8 1-0 | mainlib |
| 20.98 | 2H-1-BENZOPYRAN-2-ONE, 8-METHOXY- | 0.77 | 738 | C10H8O3 | 176 | 2445-8 1-0 | WileyRegi stry8e |
| 20.98 | 1,6-Pentalenedione, hexahydro-6a-(2-propynyl)-, cis- | 0.77 | 689 | C11H12O2 | 176 | 92485-8 7-5 | mainlib |
| 20.98 | 1,6-PENTALENEDIONE, HEXAHYDRO-6A-(2-PROPYNYL) -, CIS- | 0.77 | 689 | C11H12O2 | 176 | 92485-8 7-5 | WileyRegi stry8e |
| 20.98 | N'-(2-HYDROXY-3-ALLYLBENZ YLIDENE)-2-BENZAMIDOPROP ANHYDRAZIDE | 0.77 | 685 | C20H21N3O3 | 351 | NA | WileyRegi stry8e |
| 21.15 | 5-BENZOFURANACETIC ACID, 6-ETHENYL-2,4,5,6,7,7A-HEXAH YDRO-3,6-DIMETHYL-a-METHY LENE-2-OXO-, METHYL ESTER | 0.78 | 730 | C16H20O4 | 276 | 19892-1 9-4 | WileyRegi stry8e |
| 21.15 | 1H-INDOL-5-OL, 3-(2-AMINOETHYL)- | 0.78 | 741 | C10H12N2O | 176 | 50-67-9 | WileyRegi stry8e |
| 21.15 | Aromadendrene oxide-(2) | 0.78 | 728 | C15H24O | 220 | NA | mainlib |
| 21.15 | AROMADENDRENOXID-(2) | 0.78 | 728 | C15H24O | 220 | NA | WileyRegi stry8e |
| 21.15 | ALLOAROMADENDRENOXID-(1) | 0.78 | 722 | C15H24O | 220 | 85710-3 9-0 | WileyRegi stry8e |
| 22.64 | 3à,4à,9à,11-Diepoxymuurolan-10-ol | 0.65 | 739 | C15H24O3 | 252 | NA | mainlib |
| 22.64 | ALLOAROMADENDRENOXID-(1) | 0.65 | 727 | C15H24O | 220 | NA | WileyRegi stry8e |
| 22.64 | Alloaromadendrene oxide-(1) | 0.65 | 726 | C15H24O | 220 | NA | mainlib |
| 22.64 | 2,3-Dehydro-4-oxo-à-ionol | 0.65 | 745 | C13H18O2 | 206 | NA | mainlib |
| 22.64 | Curcumenol | 0.65 | 674 | C15H22O2 | 234 | 19431-8 4-6 | mainlib |
| 23.37 | ETHANOL, 2-(9-OCTADECENYLOXY)-, (Z)- | 3.51 | 800 | C20H40O2 | 312 | 5353-2 5-3 | WileyRegi stry8e |
| 23.37 | Ethanol, 2-(9-octadecenyloxy)-, (Z)- | 3.51 | 798 | C20H40O2 | 312 | 5353-2 5-3 | mainlib |
| 23.37 | 13-Heptadecyn-1-ol | 3.51 | 784 | C17H32O | 252 | 56554-7 7-9 | mainlib |
| 23.37 | 13-HEPTADECYN-1-OL | 3.51 | 784 | C17H32O | 252 | 56554-7 7-9 | WileyRegi stry8e |
| 23.37 | Octadecanal | 3.51 | 880 | C18H36O | 268 | 638-66 -4 | mainlib |
| 24.03 | 1-Heptatriacontanol | 0.44 | 795 | C37H76O | 536 | 105794 -58-9 | mainlib |
| 24.03 | Spiro[4.5]decan-7-one, 1,8-dimethyl-8,9-epoxy-4-isopropyl- | 0.44 | 774 | C15H24O2 | 236 | 61050-9 1-7 | mainlib |
| 24.03 | SPIRO[4.5]DECAN7-ONE, 1,8-DIMETHYL-8,9-EPOXY-4-ISO PROPYL- | 0.44 | 774 | C15H24O2 | 236 | NA | WileyRegi stry8e |
| 24.03 | SPIRO[7H-CYCLOHEPTA[B]FUR AN-7,2'(5'H)-FURAN]-5',5(3H)-DIO NE, OCTAHYDRO-8-HYDROXY-4,8-DIMETHYL-3-METHYLENE-, [3AS-(3Aà,6à,7à,8à,8Aà)]- | 0.44 | 767 | C15H20O5 | 280 | 3533-4 7-9 | WileyRegi stry8e |
| 24.03 | 2-[5-(2,2-Dimethyl-6-methylene-cyc lohexyl)-3-methyl-pent-2-enyl]-[1,4] benzoquinone | 0.44 | 734 | C21H28O2 | 312 | NA | mainlib |
| 24.18 | Cholestan-3-ol, 2-methylene-, (3à,5à)- | 2.42 | 821 | C28H48O | 400 | 22599-9 6-8 | mainlib |
| 24.18 | CHOLESTAN-3-OL, 2-METHYLENE-, (3à,5à)- | 2.42 | 820 | C28H48O | 400 | 22599-9 6-8 | WileyRegi stry8e |
| 24.18 | Ethanol, 2-(9-octadecenyloxy)-, (Z)- | 2.42 | 781 | C20H40O2 | 312 | 5353-2 5-3 | mainlib |
| 24.18 | ETHANOL, 2-(9-OCTADECENYLOXY)-, (Z)- | 2.42 | 781 | C20H40O2 | 312 | 5353-2 5-3 | WileyRegi stry8e |
| 24.18 | 17-Octadecynoic acid | 2.42 | 782 | C18H32O2 | 280 | 34450-1 8-5 | mainlib |
| 24.35 | Picrotoxin | 0.50 | 780 | C15H16O6 | 292 | 124-87 -8 | mainlib |
| 24.35 | [1,1'-BICYCLOPROPYL]-2-OCTAN OIC ACID, 2'-HEXYL-, METHYL ESTER | 0.50 | 789 | C21H38O2 | 322 | 56687-6 8-4 | WileyRegi stry8e |
| 24.35 | [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester | 0.50 | 790 | C21H38O2 | 322 | 56687-6 8-4 | mainlib |
| 24.35 | E,E,Z-1,3,12-Nonadecatriene-5,14-diol | 0.50 | 727 | C19H34O2 | 294 | NA | mainlib |
| 24.35 | cis-Z-à-Bisabolene epoxide | 0.50 | 744 | C15H24O | 220 | NA | mainlib |
| 24.66 | 13-Heptadecyn-1-ol | 0.59 | 771 | C17H32O | 252 | 56554-7 7-9 | mainlib |
| 24.66 | 13-HEPTADECYN-1-OL | 0.59 | 771 | C17H32O | 252 | 56554-7 7-9 | WileyRegi stry8e |
| 24.66 | Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy- | 0.59 | 756 | C30H52O2 | 444 | NA | mainlib |
| 24.66 | TRICYCLO[20.8.0.0(E7,16]TRIAC ONTAN, 1(22),7(16)-DIEPOXY- | 0.59 | 756 | C30H52O2 | 444 | NA | WileyRegi stry8e |
| 24.66 | E,E,Z-1,3,12-Nonadecatriene-5,14-diol | 0.59 | 736 | C19H34O2 | 294 | NA | mainlib |
| 25.01 | 1-Heptatriacontanol | 0.71 | 792 | C37H76O | 536 | 105794 -58-9 | mainlib |
| 25.01 | Cholestan-3-ol, 2-methylene-, (3à,5à)- | 0.71 | 830 | C28H48O | 400 | 22599-9 6-8 | mainlib |
| 25.01 | CHOLESTAN-3-OL, 2-METHYLENE-, (3à,5à)- | 0.71 | 829 | C28H48O | 400 | 22599-9 6-8 | WileyRegi stry8e |
| 25.01 | 13-Heptadecyn-1-ol | 0.71 | 772 | C17H32O | 252 | 56554-7 7-9 | mainlib |
| 25.01 | 13-HEPTADECYN-1-OL | 0.71 | 770 | C17H32O | 252 | 56554-7 7-9 | WileyRegi stry8e |
| 25.10 | 1,25-Dihydroxyvitamin D3, TMS derivative | 0.47 | 782 | C30H52O3Si | 488 | 55759-9 4-9 | mainlib |
| 25.10 | 9,10-SECOCHOLESTA-5,7,10(19)-T RIENE-1,3-DIOL, 25-[(TRIMETHYLSILYL)OXY]-, (3à,5Z,7E)- | 0.47 | 782 | C30H52O3Si | 488 | 55759-9 4-9 | WileyRegi stry8e |
| 25.10 | 2-ACETYL-3-(2-CINNAMIDO)ETH YL-7-METHOXYINDOLE | 0.47 | 768 | C22H22N2O3 | 362 | NA | WileyRegi stry8e |
| 25.10 | TRIDEUTERIOMETHYL 10-EPOXY-7-ETHYL-3,11-DIMET HYLTRIDECA-2,6-DIENOATE | 0.47 | 759 | C18H27D3O3 | 297 | 56805-1 1-9 | WileyRegi stry8e |
| 25.10 | 9-OCTADECENOIC ACID (Z)- | 0.47 | 734 | C18H34O2 | 282 | 112-80 -1 | WileyRegi stry8e |
| 25.64 | PENTADECANOIC ACID, 14-METHYL-, METHYL ESTER | 1.38 | 730 | C17H34O2 | 270 | 5129-6 0-2 | WileyRegi stry8e |
| 25.64 | Oxiraneundecanoic acid, 3-pentyl-, methyl ester, cis- | 1.38 | 725 | C19H36O3 | 312 | 38520-3 0-8 | mainlib |
| 25.64 | OXIRANEUNDECANOIC ACID, 3-PENTYL-, METHYL ESTER, CIS- | 1.38 | 725 | C19H36O3 | 312 | 38520-3 0-8 | WileyRegi stry8e |
| 25.64 | OXIRANEUNDECANOIC ACID, 3-PENTYL-, METHYL ESTER, TRANS- | 1.38 | 723 | C19H36O3 | 312 | 38520-3 1-9 | WileyRegi stry8e |
| 25.64 | Oxiraneundecanoic acid, 3-pentyl-, methyl ester, trans- | 1.38 | 723 | C19H36O3 | 312 | 38520-3 1-9 | mainlib |
| 26.50 | HEXADECANOIC ACID, 2,3-DIHYDROXYPROPYL ESTER | 3.34 | 784 | C19H38O4 | 330 | 542-44 -9 | WileyRegi stry8e |
| 26.50 | PENTADECANOIC ACID | 3.34 | 778 | C15H30O2 | 242 | 1002-8 | WileyRegi |

**Table 3: GC-MS identified compounds in the methanolic extract of *Lavandula dentate***

| RT | Compound Name | Area % | MF | Molecular Formula | Molecular Weight | Cas # | Library |
|---|---|---|---|---|---|---|---|
| 26.50 | Oleic Acid | 3.34 | 810 | C18H34O2 | 282 | 112-80-1 | replib |
| 26.50 | 9-OCTADECENOIC ACID | 3.34 | 810 | C18H34O2 | 282 | NA | Wiley Registry8e |
| 26.50 | HEXADECANOIC ACID | 3.34 | 798 | C16H32O2 | 256 | 57-10-3 | Wiley Registry8e |
| 27.37 | Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate | 1.04 | 784 | C16H28O3 | 268 | NA | mainlib |
| 27.37 | 01297107001 TETRANEURIN - A - DIOL | 1.04 | 765 | C15H20O5 | 280 | NA | Wiley Registry8e |
| 27.37 | 13-HEPTADECYN-1-OL | 1.04 | 774 | C17H32O | 252 | 56554-77-9 | Wiley Registry8e |
| 27.37 | 13-Heptadecyn-1-ol | 1.04 | 774 | C17H32O | 252 | 56554-77-9 | mainlib |
| 27.37 | 1-Heptatriacontanol | 1.04 | 764 | C37H76O | 536 | 105794-58-9 | mainlib |
| 28.65 | 7,10-Octadecadienoic acid, methyl ester | 2.48 | 859 | C19H34O2 | 294 | 56554-24-6 | mainlib |
| 28.65 | 7,10-OCTADECADIENOIC ACID, METHYL ESTER | 2.48 | 858 | C19H34O2 | 294 | 56554-24-6 | Wiley Registry8e |
| 28.65 | 9,12-OCTADECADIENOIC ACID, METHYL ESTER, (E,E)- | 2.48 | 836 | C19H34O2 | 294 | 2566-97-4 | Wiley Registry8e |
| 28.65 | 9,12-Octadecadienoic acid, methyl ester, (E,E)- | 2.48 | 835 | C19H34O2 | 294 | 2566-97-4 | mainlib |
| 28.65 | 9,12-OCTADECADIENOIC ACID (Z,Z)-, METHYL ESTER | 2.48 | 830 | C19H34O2 | 294 | 112-63-0 | Wiley Registry8e |
| 28.83 | 11-Octadecenoic acid, methyl ester | 3.25 | 849 | C19H36O2 | 296 | 52380-33-3 | replib |
| 28.83 | 9-Octadecenoic acid, methyl ester, (E)- | 3.25 | 846 | C19H36O2 | 296 | 1937-62-8 | replib |
| 28.83 | METHYL 9,9-DIDEUTERO-OCTADECANOATE | 3.25 | 838 | C19H36D2O2 | 300 | 19905-64-7 | Wiley Registry8e |
| 28.95 | Oleic Acid | 1.03 | 794 | C18H34O2 | 282 | 112-80-1 | replib |
| 28.95 | 2-HYDROXY-3-[(9E)-9-OCTADECENOYLOXY]PROPYL (9E)-9-OCTADECENOATE # | 1.03 | 779 | C39H72O5 | 620 | 2465-32-9 | Wiley Registry8e |
| 28.95 | trans-13-Octadecenoic acid | 1.03 | 791 | C18H34O2 | 282 | 693-71-0 | mainlib |
| 28.95 | cis-Vaccenic acid | 1.03 | 785 | C18H34O2 | 282 | 506-17-2 | mainlib |
| 28.95 | Linoleic acid ethyl ester | 1.03 | 768 | C20H36O2 | 308 | 544-35-4 | replib |
| 29.17 | Cholestan-3-ol, 2-methylene-, (3à,5à)- | 1.18 | 849 | C28H48O | 400 | 22599-96-8 | mainlib |
| 29.17 | CHOLESTAN-3-OL, 2-METHYLENE-, (3à,5à)- | 1.18 | 848 | C28H48O | 400 | 22599-96-8 | Wiley Registry8e |
| 29.17 | E,E,Z-1,3,12-Nonadecatriene-5,14-diol | 1.18 | 768 | C19H34O2 | 294 | NA | mainlib |
| 29.17 | Ethanol, 2-(9-octadecenyloxy)-, (Z)- | 1.18 | 756 | C20H40O2 | 312 | 5353-25-3 | mainlib |
| 29.17 | Linoleic acid ethyl ester | 1.18 | 754 | C20H36O2 | 308 | 544-35-4 | replib |
| 29.62 | 9-OCTADECENOIC ACID (Z)- | 11.17 | 860 | C18H34O2 | 282 | 112-80-1 | Wiley Registry8e |
| 29.62 | 9,12-Octadecadienoyl chloride, (Z,Z)- | 11.17 | 857 | C18H31ClO | 298 | 7459-38-8 | replib |
| 29.62 | (9E,12E)-9,12-OCTADECADIENOYL CHLORIDE # | 11.17 | 857 | C18H31ClO | 298 | 7459-38-8 | Wiley Registry8e |
| 29.62 | 9,12-Octadecadienoic acid (Z,Z)- | 11.17 | 848 | C18H32O2 | 280 | 60-33-3 | replib |
| 29.62 | 9,12-OCTADECADIENOIC ACID (Z,Z)- | 11.17 | 848 | C18H32O2 | 280 | 60-33-3 | Wiley Registry8e |
| 32.86 | [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester | 0.76 | 840 | C21H38O2 | 322 | 56687-68-4 | mainlib |
| 32.86 | [1,1'-BICYCLOPROPYL]-2-OCTANOIC ACID, 2'-HEXYL-, METHYL ESTER | 0.76 | 836 | C21H38O2 | 322 | 56687-68-4 | Wiley Registry8e |
| 32.86 | Cholestan-3-ol, 2-methylene-, (3à,5à)- | 0.76 | 830 | C28H48O | 400 | 22599-96-8 | mainlib |
| 32.86 | CHOLESTAN-3-OL, 2-METHYLENE-, (3à,5à)- | 0.76 | 829 | C28H48O | 400 | 22599-96-8 | Wiley Registry8e |
| 32.86 | Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate | 0.76 | 774 | C16H28O3 | 268 | NA | mainlib |
| 33.13 | Linoleic acid ethyl ester | 0.39 | 783 | C20H36O2 | 308 | 544-35-4 | replib |
| 33.13 | E,E,Z-1,3,12-Nonadecatriene-5,14-diol | 0.39 | 790 | C19H34O2 | 294 | NA | mainlib |
| 33.13 | Z,Z-3,15-Octadecadien-1-ol acetate | 0.39 | 791 | C20H36O2 | 308 | NA | mainlib |
| 33.13 | Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy- | 0.39 | 810 | C30H52O2 | 444 | NA | mainlib |
| 33.13 | TRICYCLO[20.8.0.0E7,16]TRIACONTAN, 1(22),7(16)-DIEPOXY- | 0.39 | 810 | C30H52O2 | 444 | NA | Wiley Registry8e |
| 33.28 | 9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 0.59 | 823 | C21H40O4 | 356 | 3443-84-3 | mainlib |
| 33.28 | 9-OCTADECENOIC ACID (Z)-, 2-HYDROXY-1-(HYDROXYMETHYL)ETHYL ESTER | 0.59 | 820 | C21H40O4 | 356 | 3443-84-3 | Wiley Registry8e |
| 33.28 | Oleic Acid | 0.59 | 789 | C18H34O2 | 282 | 112-80-1 | replib |
| 33.28 | trans-9-Octadecenoic acid, pentyl ester | 0.59 | 802 | C23H44O2 | 352 | NA | mainlib |
| 33.28 | 9-Octadecenoic acid, 1,2,3-propanetriyl ester, (E,E,E)- | 0.59 | 778 | C57H104O6 | 884 | 537-39-3 | mainlib |
| 35.83 | ISOCHIAPIN B | 2.31 | 736 | C19H22O6 | 346 | NA | Wiley Registry8e |
| 35.83 | ISOCHIAPIN B %2< | 2.31 | 736 | C19H26O6 | 350 | NA | Wiley Registry8e |
| 35.83 | 3',8,8'-Trimethoxy-3-piperidyl-2,2'-binaphthalene-1,1',4,4'-tetrone | 2.31 | 759 | C28H25NO7 | 487 | 127611-84-1 | mainlib |
| 35.83 | 4H-1-BENZOPYRAN-4-ONE, 2-(3,4-DIHYDROXYPHENYL)-6,8-DI-à-D-GLUCOPYRANOSYL-5,7-DIHYDROXY- | 2.31 | 716 | C27H30O16 | 610 | 29428-58-8 | Wiley Registry8e |
| 35.83 | 1,2-BENZENEDICARBOXYLIC ACID | 2.31 | 757 | C24H38O4 | 390 | 117-81-7 | Wiley Registry8e |
| 38.80 | ISOCHIAPIN B | 0.82 | 782 | C19H22O6 | 346 | NA | Wiley Registry8e |
| 38.80 | ISOCHIAPIN B %2< | 0.82 | 782 | C19H26O6 | 350 | NA | Wiley Registry8e |
| 38.80 | DOTRIACONTANE | 0.82 | 790 | C32H66 | 450 | 544-85-4 | Wiley Registry8e |
| 38.80 | 4H-1-BENZOPYRAN-4-ONE, 2-(3,4-DIMETHOXYPHENYL)-3,5-DIHYDROXY-7-METHOXY- | 0.82 | 758 | C18H16O7 | 344 | 6068-80-0 | Wiley Registry8e |
| 38.80 | 1,25-Dihydroxyvitamin D3, TMS derivative | 0.82 | 804 | C30H52O3Si | 488 | 55759-94-9 | mainlib |
| 39.83 | ISOCHIAPIN B | 1.08 | 799 | C19H22O6 | 346 | NA | Wiley Registry8e |
| 39.83 | ISOCHIAPIN B %2< | 1.08 | 799 | C19H26O6 | 350 | NA | Wiley Registry8e |
| 39.83 | DOTRIACONTANE | 1.08 | 800 | C32H66 | 450 | 544-85-4 | Wiley Registry8e |
| 39.83 | 4H-1-BENZOPYRAN-4-ONE, 2-(3,4-DIHYDROXYPHENYL)-6,8-DI-à-D-GLUCOPYRANOSYL-5,7-DIHYDROXY- | 1.08 | 760 | C27H30O16 | 610 | 29428-58-8 | Wiley Registry8e |
| 40.50 | ETHYL ISO-ALLOCHOLATE | 0.87 | 767 | C26H44O5 | 436 | NA | Wiley Registry8e |
| 40.50 | Ethyl iso-allocholate | 0.87 | 769 | C26H44O5 | 436 | NA | mainlib |
| 40.50 | 1-Heptatriacontanol | 0.87 | 799 | C37H76O | 536 | 105794-58-9 | mainlib |
| 40.50 | 01297107001 TETRANEURIN - A - DIOL | 0.87 | 794 | C15H20O5 | 280 | NA | Wiley Registry8e |
| 40.50 | 2-HYDROXY-3-[(9E)-9-OCTADECENOYLOXY]PROPYL (9E)-9-OCTADECENOATE # | 0.87 | 733 | C39H72O5 | 620 | 2465-32-9 | Wiley Registry8e |
| 41.03 | ISOCHIAPIN B | 1.28 | 778 | C19H22O6 | 346 | NA | Wiley Registry8e |
| 41.03 | ISOCHIAPIN B %2< | 1.28 | 778 | C19H26O6 | 350 | NA | Wiley Registry8e |
| 41.03 | Ethyl iso-allocholate | 1.28 | 770 | C26H44O5 | 436 | NA | mainlib |
| 41.03 | ETHYL ISO-ALLOCHOLATE | 1.28 | 770 | C26H44O5 | 436 | NA | Wiley Registry8e |
| 41.03 | 1-Heptatriacontanol | 1.28 | 808 | C37H76O | 536 | 105794-58-9 | mainlib |
| 41.73 | ISOCHIAPIN B | 2.39 | 791 | C19H22O6 | 346 | NA | Wiley Registry8e |
| 41.73 | ISOCHIAPIN B %2< | 2.39 | 791 | C19H26O6 | 350 | NA | Wiley Registry8e |
| 41.73 | DOTRIACONTANE | 2.39 | 800 | C32H66 | 450 | 544-85-4 | Wiley Registry8e |
| 41.73 | 4H-1-BENZOPYRAN-4-ONE, 2-(3,4-DIMETHOXYPHENYL)-3,5-DIHYDROXY-7-METHOXY- | 2.39 | 772 | C18H16O7 | 344 | 6068-80-0 | Wiley Registry8e |
| 41.73 | 4H-1-BENZOPYRAN-4-ONE, 2-(3,4-DIHYDROXYPHENYL)-6,8-DI-à-D-GLUCOPYRANOSYL-5,7-DIHYDROXY- | 2.39 | 735 | C27H30O16 | 610 | 29428-58-8 | Wiley Registry8e |
| 42.19 | 1-Heptatriacontanol | 0.85 | 805 | C37H76O | 536 | 105794-58-9 | mainlib |
| 42.19 | Betulin | 0.85 | 721 | C30H50O2 | 442 | 473-98-3 | replib |
| 42.19 | 03027205002 FLAVONE 4'-OH,5-OH,7-DI-O-GLUCOSIDE | 0.85 | 718 | C27H30O15 | 594 | NA | Wiley Registry8e |
| 42.19 | LUP-20(29)-ENE-3,28-DIOL, (3à)- | 0.85 | 776 | C30H50O2 | 442 | 473-98-3 | Wiley Registry8e |
| 42.19 | 7,10,13-Eicosatrienoic acid, methyl ester | 0.85 | 733 | C21H36O2 | 320 | 30223-51-9 | replib |
| 42.32 | 1-Heptatriacontanol | 0.71 | 811 | C37H76O | 536 | 105794-58-9 | mainlib |
| 42.32 | STIGMAST-5-EN-3-OL, (3à,24S)- | 0.71 | 738 | C29H50O | 414 | 83-47-6 | Wiley Registry8e |
| 42.32 | Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy- | 0.71 | 792 | C30H52O2 | 444 | NA | mainlib |
| 42.32 | TRICYCLO[20.8.0.0E7,16]TRIACONTAN, 1(22),7(16)-DIEPOXY- | 0.71 | 792 | C30H52O2 | 444 | NA | Wiley Registry8e |
| 42.32 | 7,10,13-Eicosatrienoic acid, methyl ester | 0.71 | 732 | C21H36O2 | 320 | 30223-51-9 | replib |
| 42.56 | 1-Heptatriacontanol | 1.08 | 801 | C37H76O | 536 | 105794-58-9 | mainlib |
| 42.56 | STIGMAST-5-EN-3-OL, (3à,24S)- | 1.08 | 757 | C29H50O | 414 | 83-47-6 | Wiley Registry8e |
| 42.56 | 9,12-OCTADECADIENOIC ACID (Z,Z)-, 2,3-BIS[(TRIMETHYLSILYL)OXY]PROPYL ESTER | 1.08 | 757 | C27H54O4Si2 | 498 | 54284-45-6 | Wiley Registry8e |
| 42.56 | Ursodeoxycholic acid | 1.08 | 725 | C24H40O4 | 392 | 128-13-2 | mainlib |
| 42.56 | 03027205002 FLAVONE 4'-OH,5-OH,7-DI-O-GLUCOSIDE | 1.08 | 708 | C27H30O15 | 594 | NA | Wiley Registry8e |
| 42.97 | Ethyl iso-allocholate | 1.31 | 764 | C26H44O5 | 436 | NA | mainlib |
| 42.97 | ETHYL ISO-ALLOCHOLATE | 1.31 | 764 | C26H44O5 | 436 | NA | Wiley Registry8e |
| 42.97 | 1-Heptatriacontanol | 1.31 | 791 | C37H76O | 536 | 105794-58-9 | mainlib |
| 42.97 | 01297107001 TETRANEURIN - A - DIOL | 1.31 | 782 | C15H20O5 | 280 | NA | Wiley Registry8e |
| 42.97 | Tricyclo[20.8.0.0(7,16)]triacontane, 1(22),7(16)-diepoxy- | 1.31 | 780 | C30H52O2 | 444 | NA | mainlib |
| 43.07 | Ethyl iso-allocholate | 1.31 | 779 | C26H44O5 | 436 | NA | mainlib |
| 43.07 | ETHYL ISO-ALLOCHOLATE | 1.31 | 779 | C26H44O5 | 436 | NA | Wiley Registry8e |
| 43.07 | 1-Heptatriacontanol | 1.31 | 800 | C37H76O | 536 | 105794-58-9 | mainlib |
| 43.07 | 01297107001 TETRANEURIN - A - DIOL | 1.31 | 790 | C15H20O5 | 280 | NA | Wiley Registry8e |
| 43.07 | 03027205002 FLAVONE 4'-OH,5-OH,7-DI-O-GLUCOSIDE | 1.31 | 720 | C27H30O15 | 594 | NA | Wiley Registry8e |
| 45.05 | Betulinaldehyde | 15.13 | 808 | C30H48O2 | 440 | 13159-28-9 | mainlib |
| 45.05 | Betulin | 15.13 | 783 | C30H50O2 | 442 | 473-98-3 | replib |
| 45.05 | Lupeol | 15.13 | 804 | C30H50O | 426 | 545-47-1 | replib |
| 45.05 | Propanoic acid, 2-methyl-, (dodecahydro-6a-hydroxy-9a-methyl-3-methylene-2,9-dioxoazuleno[4,5-b]furan-6-yl)methyl ester, [3aS-(3aâ,6à,6aâ,9aâ,9bà)]- | 15.13 | 757 | C19H26O6 | 350 | 33649-17-1 | mainlib |
| 45.05 | PROPANOIC ACID, 2-METHYL-, (DECAHYDRO-6A-HYDROXY-9 | 15.13 | 757 | C19H26O6 | 350 | 33649-17-1 | Wiley Registry8e |

major constituents identified was linalool, which is consistent with previous studies on *Lavandula* species (Bilia *et al*., 2014). Linalool has been extensively studied for its pharmacological properties, including its antimicrobial (Faleiro *et al*., 2003) and anxiolytic effects (Linck *et al*., 2009).

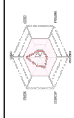
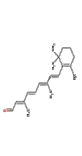
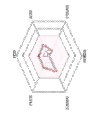
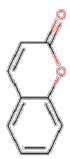
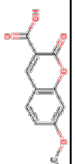
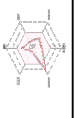
Moreover, the presence of Chromen-2-one was detected in the *Lavandula dentata* extract. Chromenes, also known as chromanones or chromones, represent an important class of heterocyclic compounds with diverse biological activities (Zhang *et al*., 2016). These compounds are characterized by their structural motif comprising a benzene ring fused to a cyclic ether ring. Chromenes exhibit a wide range of pharmacological properties, making them valuable targets for drug discovery and development. For instance, several studies have highlighted the anticancer potential of chromenes due to their ability to inhibit various cancer cell proliferation pathways (Zhou *et al*., 2019).

Additionally, chromenes have been reported to possess antioxidant properties, which can play a crucial role in combating oxidative stress-related diseases such as cardiovascular disorders and neurodegenerative conditions (Zhang *et al*., 2016). Furthermore, chromenes have attracted significant attention in the field of medicinal chemistry owing to their diverse biological activities. Research efforts have focused on synthesizing novel chromene derivatives with enhanced pharmacological profiles (Xu *et al*., 2020). These derivatives often undergo structural modifications to optimize their drug-like properties, such as improving solubility, bioavailability and target specificity.

Additionally, retinal was identified in the *Lavandula dentata* leaves extract. Retinal, a derivative of vitamin A, plays a crucial role in vision by serving as the light-absorbing chromophore in visual pigments (Palczewski, 2006). It is a vital component of the visual cycle, where it undergoes photoisomerization upon absorbing light to initiate signal transduction in photoreceptor cells. In addition to its role in vision, retinal also participates in non-visual processes, including the regulation of circadian rhythms (Buhr *et al*., 2015). Melanopsin-containing retinal ganglion cells in the retina utilize retinal as a chromophore to detect light and transmit signals to the brain's suprachiasmatic nucleus, thereby synchronizing the body's internal clock with the day-night cycle. Furthermore, retinal is essential for maintaining the health and integrity of retinal tissue. Deficiencies in retinal metabolism or transport can lead to retinal degenerative diseases such as retinitis pigmentosa and age-related macular degeneration (Sparrow *et al*., 2010). Understanding the biochemical pathways involving retinal metabolism is crucial for developing therapeutic interventions to treat these blinding disorders.

Furthermore, the GC-MS analysis detected the presence of Cumarin-3-carboxylic acid, 7-methoxy. Cumarin-3-carboxylic acid, 7-methoxy, also known as methoxycoumarin or 7-methoxycoumarin, is a derivative of

**Table 4:** Physicochemical properties of selected compounds of LE.

| Molecule | Molecule 2D structure | Radar chart | MW | Number of heavy atoms | Number of aromatic heavy atoms | Fraction Csp3 | Number of rotatable bonds | Number of H-bond acceptors | Number of H-bond donors | MR | TPSA (topological polar surface area) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Linalool |  |  | 154.25 | 11 | 0 | 0.6 | 4 | 1 | 1 | 50.44 | 20.23 |
| Retinal |  |  | 284.44 | 21 | 0 | 0.45 | 5 | 1 | 0 | 93.71 | 17.07 |
| chromene-2-one |  |  | 146.14 | 11 | 10 | 0 | 0 | 2 | 0 | 42.48 | 30.21 |
| 7-Methoxy-2-oxo -2H-chromene-3-carboxylic acid |  |  | 220.18 | 16 | 10 | 0.09 | 2 | 5 | 1 | 55.94 | 76.74 |

MW: Molecular weight; MR: Molecular refractivity.

coumarin with a methoxy substituent at the 7-position of the aromatic ring. This compound belongs to the broader class of coumarin derivatives and has garnered attention for its potential pharmacological activities and diverse applications in medicinal chemistry. Studies have indicated that Cumarin-3-carboxylic acid, 7-methoxy, possesses notable biological properties, including antioxidant and anti-inflammatory effects. These properties make it a promising

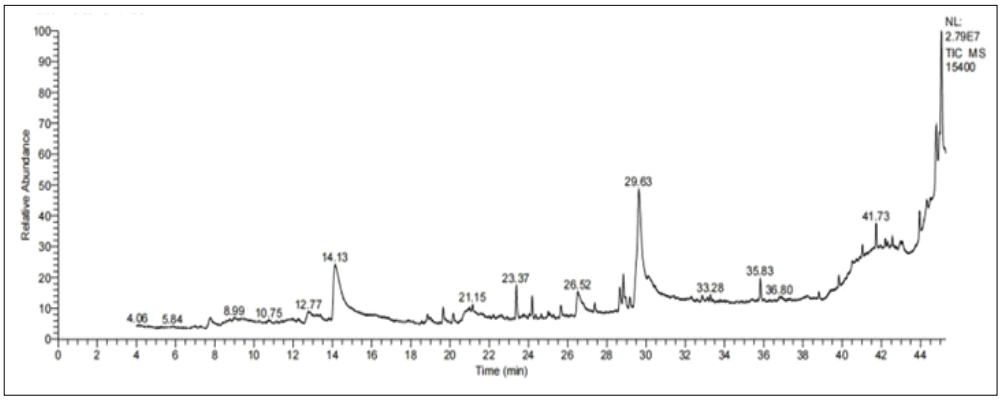



**Fig 1:** Chromatogram of methanolic extract of *Lavandula dentata*.

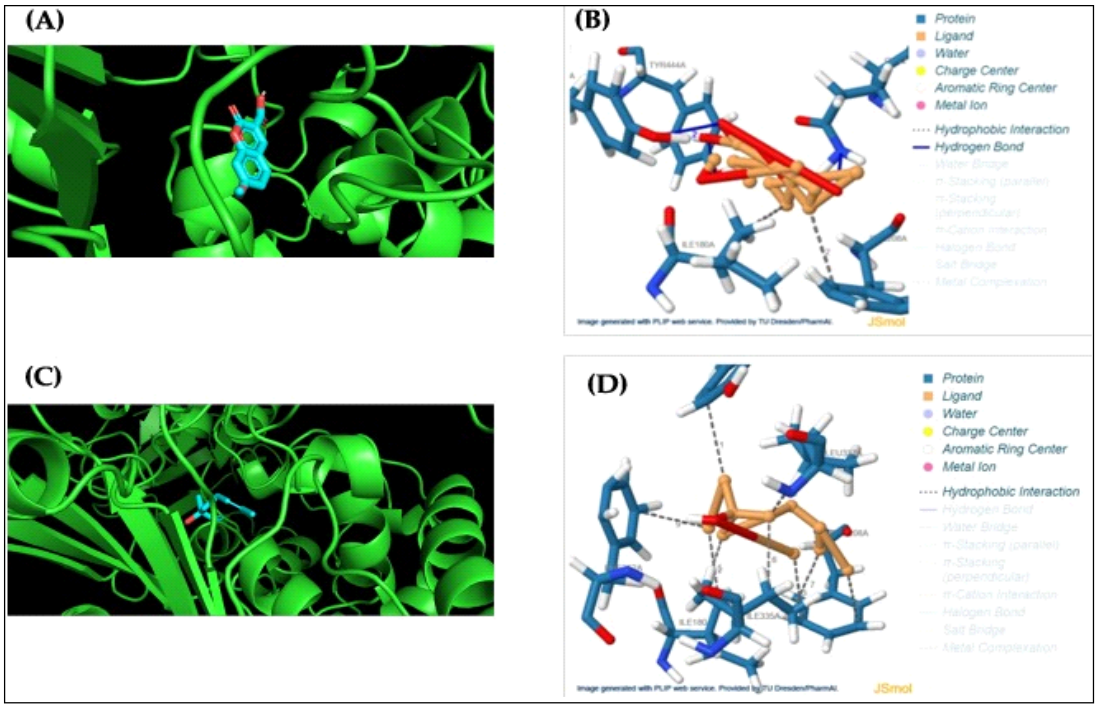



**Fig 2:** 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid (A, using PyMOL and B, using PLIP) and linalool (C, using PyMOL and D, using PLIP) docking Monoamine oxidase a showing the interactions.

**Table 5:** Lipophilicity of selected compounds of LE.

| Molecule | Log *Po/w* (iLogP) | XLogP3 | WLogP | MLogP | Silicos-IT Log P | Consensus Log P |
|---|---|---|---|---|---|---|
| Linalool | 2.7 | 2.97 | 2.67 | 2.59 | 2.35 | 2.66 |
| Retinal | - | - | 5.72 | - | - | - |
| chromene-2-one | 1.75 | 1.39 | 1.79 | 1.65 | 2.5 | 1.82 |
| 7-Methoxy-2-oxo-2H-chromene -3-carboxylic acid | 1.42 | 2.17 | 1.5 | 0.95 | 1.81 | 1.57 |

(-) means unknown data.

**Table 6:** Water Solubility of selected compounds of LE.

| Molecule | Log S (ESOL) | Solubility (ESOL) (mg/ml) | Solubility (ESOL) (mol/l) | ESOL class | Log S (Ali) | Solubility (Ali) (mg/ml) | Solubility (Ali) (mol/l) | Ali class | Log S (Silicos-IT) | Solubility (Silicos-IT) (mg/ml) | Silicos-IT solubility (mol/l) | Silicos-IT class |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Linalool | -2.4 | 6.09e-01 | 3.95e-03 | Soluble | -3.06 | 1.35e-01 | 8.75e-04 | Soluble | -1.84 | 2.20e+00 | 1.43e-02 | Soluble |
| Retinal | - | - | - | - | - | - | - | - | - | - | - | - |
| chromene-2-one | -2.29 | 7.42E-01 | 5.08E-03 | Soluble | -1.63 | 3.44E+00 | 2.35E-02 | Very soluble | -3.59 | 3.77E-02 | 2.58E-04 | Soluble |
| 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid | -2.9 | 2.75E-01 | 1.25E-03 | Soluble | -3.41 | 8.48E-02 | 3.85E-04 | Soluble | -3.12 | 1.67E-01 | 7.59E-04 | Soluble |

(-) means unknown data.

**Table 7:** Pharmacokinetics, drug-likeness and medicinal chemistry of selected compounds of LE.

| Molecule | Gastrointestinal (GI) absorption | Blood-brain barrier (BBB) permeant | Log Kp (cm/s) | Lipinski violations number | Bioavailability score | PAINS alerts | Brenk alerts | Leadlikeness violations | Synthetic accessibility |
|---|---|---|---|---|---|---|---|---|---|
| Linalool | High | Yes | -5.13 | 0 | 0.55 | 0 | 1 | 1 | 2.74 |
| Retinal | - | Yes | - | - | - | 0 | 0 | - | - |
| chromene-2-one | High | Yes | -6.2 | 0 | 0.55 | 0 | 1 | 1 | 2.74 |
| 7-Methoxy-2-oxo-2H-chromene -3-carboxylic acid | High | No | -6.1 | 0 | 0.56 | 0 | 1 | 1 | 2.57 |

(-) means unknown data; PAINS, pan-assay interference compounds.

candidate for the development of therapeutic agents targeting oxidative stress-related diseases and inflammatory conditions (Borges *et al*., 2016). The presence of the methoxy group at the 7-position may contribute to its antioxidant activity by enhancing its ability to scavenge free radicals and mitigate oxidative damage. Moreover, Cumarin-3-carboxylic acid, 7-methoxy has been investigated for its potential anticancer properties. Research suggests that certain methoxycoumarin derivatives exhibit cytotoxic effects against cancer cells and may hold promise as anticancer agents through mechanisms such as induction of apoptosis and inhibition of proliferation (Yang *et al*., 2015). The structural modification of coumarin to incorporate a methoxy group at the 7-position could influence its interactions with cellular targets involved in cancer progression, thereby enhancing its therapeutic efficacy. Furthermore, methoxycoumarin derivatives have been explored for their antimicrobial activities. Studies have demonstrated the antibacterial and antifungal properties of certain methoxycoumarin derivatives, indicating their potential as antimicrobial agents for combating infectious diseases (Lee *et al*., 2019). The presence of the methoxy group may contribute to the compound's ability to disrupt microbial cell membranes or interfere with essential metabolic processes, thereby exerting antimicrobial effects.

Four phytocompounds (linalool, retinal, chromene-2-one and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid) were analyzed for Amine Oxidase A docking studies. Their physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry are found in Tables 4-7. Retinal was excluded according to missing calculated parameters. Linalool, chromene-2-one and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid met Lipinski's conditions, which is considered to predict optimal drug-like character. They reported no Lipinski's violations that suggested these are orally bioavailable drugs. It is reported that selected compounds have low lipophilicity, good gastrointestinal absorption and blood-brain barrier permeability (except for 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid) and bioavailability (Daina *et al*., 2014).

In ProTox-II, linalool and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid are assumed to be non-toxic with their predicted toxicity class and LD50 2200 mg/kg

**Table 8:** Interactions of 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid and amine oxidase A docking site.

| Hydrophobic interactions | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Index | Residue | Amino acid | Distance | Ligand atom | Protein atom | | | |
| 1 | 180A | ILE | 3.41 | 8205 | 2717 | | | |
| 2 | 208A | PHE | 3.26 | 8209 | 3167 | | | |
| Hydrogen Bonds | | | | | | | | |
| Index | Residue | Amino acid | Distance H-A | Distance D-A | Donor angle | Protein donor? | Side chain | Donor atom | Acceptor atom |
| 1 | 215A | GLN (Glutamine) | 3.00 | 3.79 | 123.77 | √ | √ | 3257 [Nam] | 8217 [O3] |
| 2 | 407A | TYR (Tyrosine) | 2.05 | 3.10 | 145.56 | √ | √ | 6347 [O] | 8214 [O2] |
| 3 | 444A | TYR | 2.92 | 3.55 | 113.03 | √ | √ | 6931 [O3] | 8215 [O.co2] |
| 4 | 444A | TYR | 3.31 | 3.55 | 108.53 | X | √ | 8215 [O.co2] | 6931 [O3] |

**Table 9:** Interactions of linalool and monoamine oxidase A docking site.

| Hydrophobic interactions | | | | | |
|---|---|---|---|---|---|
| Index | Residue | Amino acid | Distance | Ligand atom | Protein atom |
| 1 | 69A | TYR (Tyrosine) | 3.61 | 8203 | 860 |
| 2 | 180A | ILE (Isoleucine) | 3.57 | 8204 | 2717 |
| 3 | 208A | PHE (Phenylalanine) | 3.65 | 8211 | 3170 |
| 4 | 208A | PHE | 3.62 | 8210 | 5186 |
| 5 | 335A | ILE | 3.70 | 8205 | 5185 |
| 6 | 335A | ILE | 3.45 | 8206 | 5187 |
| 7 | 335A | ILE | 3.57 | 8209 | 5218 |
| 8 | 337A | LEU (Leucine) | 3.62 | 8206 | 5430 |
| 9 | 352A | PHE | 3.87 | 8204 | 5430 |

(Class: 5) and 200 mg/kg (Class: 3), respectively. Linalool is assumed to be safer than 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid because it is inactive against hepato-, neuro-, nephro-, cardio-, cyto-, immuno-, respiratory toxicity, carcino- and mutagenicity.

For molecular docking: Linalool and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid were docked, separately, with the receptor Amine Oxidase A. The docking scores of linalool and 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid are -24.4 and -33.7, respectively, with the receptor protein. Both are docked with nearly identical co-crystallized ligand Harmine binding site to receptor protein. However, linalool appears to be more stable in the docking site due to the presence of nine hydrophobic interactions with the receptor protein in comparison with only two hydrophobic interactions for 7-Methoxy-2-oxo-2H-chromene-3-carboxylic acid (Table 8 and 9, Fig 2). The *in silico* and docking computational results suggested that linalool could be a promise MAO-A inhibitor.

Computational analysis plays a critical role in the identification and development of new drugs with better therapeutic effects. Cheminformatics and molecular modeling have long been used to discover and develop better drug therapies (Noorjahan and Saranya, 2018). As part of standard drug discovery processes, in silico modeling is now an integral component. These methods aid in discovering new medications or improving the therapeutic efficacy of a chemical series in early drug development (Kumar *et al*., 2024; Stanzione *et al*., 2021). Linalool's potential activity in the central nervous system has been studied for its mechanism of antidepressant action through monoaminergic pathways. New studies have expanded knowledge about its interaction with different targets and pathways, making it a promising natural compound for treating depression (Dos Santos *et al*., 2022). According to the present results, linalool could have a crucial role in the treatment of different neurodegenerative disorders through its highly effective MAO-A inhibition. Therefore, further *in vitro* and *in vivo* studies are needed to verify our assumption and report its mechanism pathway.

## CONCLUSION

In conclusion, the GC-MS analysis of the methanolic extract of *Lavandula dentata* leaves revealed the presence of various bioactive compounds including linalool, retinal, chromene-2-one and Cumarin-3-carboxylic acid, 7-methoxy. These compounds have been associated with diverse pharmacological properties, suggesting the therapeutic potential of *Lavandula dentata* extract in medicine and pharmaceutical applications. Linalool has an effective inhibitory action on MAO-A according to the present *in silico* and docking analysis that could be a promising safe therapeutic drug for various neurodegenerative diseases. More studies are thus recommended to shed more light on the pharmacological and medical properties of *Lavandula dentata*.

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### Author contributions

The authors contributed to the practical part, writing the original draft, editing and accepting the final version of this article.

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### Conflict of interest

The authors declare no conflict of interest.

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