Profile of bioactive compounds in *Rosmarinus officinalis*

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INTRODUCTION

Rosemary (*Rosmarinus officinalis* L.), belongs to family Lamiaceae, is aromatic, evergreen, usually erect, bushy shrub up to 2m tall and wide. Stem indistinctly quadrangular finely grey pubescent. Leaves opposite, tufted on the branches, sessile to short, petiolate, blade linear, 1-5cmx1-2mm, base attenuate, margin entire but revolute, apex obtuse, leathery, dark glossy, sea green and sub glabrous above, white felted tomentose beneath, aromatically fragrant when crushed. Inflorescence Racemose, axillary 5-10 flowered, 0.5-2.5 cm long, terminating short lateral branches, pedicle 2-5mm long, calyx campanulate, 2-lipped, 5-6mm long, densely stellate tomentose, upper lip small and 3 dentate, lower lip 2-lobed, corolla tabular, 2 lipped, 10- 13 mm long, pale blue or white, upper lip or curved, 2-lobed, ovate, about 4mm long, lower lip 3-lobed above 7mm long, with large concave middle lobe; 2 anterior stamens perfect, 7-8 mm long, ascending under the base of the upper lip, two posterior stamens reduced to hardly visible staminodes, pistil with deeply 4-parite ovary style incurved, 1.5 cm long ending into 2 short, unequal branches with stigma. Fruit composed of 4sub-globose to obovoid nutlets, above 2mm long, glabrous and smooth; Flowering – Nov - Jan ¹,².

Since antiquity foliage is used as a common household culinary spice for flavouring. Rosemary extracts, derived from leaves, are used as flavouring and antioxidant agents in food processing and cosmetics. Rosemary has been used in traditional and complementary alternative medicine for its digestive, tonic, astringent, diuretic, and diaphoretic properties. It has been linked to a broad range of beneficial health benefits³.

Main constituents of ROEO are camphor (5.0-21%), 1,8-cineole (15-55%), α-pinene (9.0-26%), bornol (1.5-5.0%), camphene (2.5-12%), β-pinene (2.0-9.0%) and limonene (1.5-5.0%) in proportions that vary according to the vegetative stage and bioclimatic conditions⁴. Rosemary has long been used in traditional medicine to cure a variety of ailments⁵. Phytochemicals in *R. officinalis* include rosmarinic acid, camphor, caffeic acid, ursolic acid, betulinic acid, carnosic acid and carnosol⁶. ROEO composed of phenolic compounds, di and triterpenes and essential oils. In traditional medicine ROEO is used to treat wounds, rashes, headache, dyspepsia,
circulation problems, and as expectorant, diuretic and anti-spasmodic in treatment of renal colic which is attributed to the class of chemical compounds. Polyphenols are antioxidants primarily responsible for fruit colouring, and are classified as phenolic acids, flavonoids and non-flavonoids. Epidemiology evidence indicates that a diet rich in antioxidant fruits and vegetables significantly reduces the risk of many oxidative stress related diseases viz. cancers, diabetes and cardiovascular diseases (CVD). In addition to their antioxidant properties, ROEO play a very important role in plant defences against herbivores, pathogens and predators; therefore, used to control infectious agents in humans. Polyphenols in ROEO are apigenin, diosmin, luteolin, genkwanin and phenolic acids (>3%), especially rosmarinic acid, chlorogenic acid and caffeic acid. Furthermore, biological activities exhibited by phenolic acids in There are numerous epidemiological and experimental evidences present describing the protective role of phenolic acids in degenerative diseases such as cardiovascular, cancer, diabetes, inflammation and many more. The ability of plant secondary metabolites depends on the bioavailability which accounts for the proportion of their absorption, digestion, and metabolism after entering in the circulation system.

**MATERIALS AND METHODS**

Collection of Plant material: *Rosmarinus officinalis* L. (Rosemary) leaves were collected from Palani Hills, Western Ghats (2000 m above the mean sea level), and identity of the plant was confirmed by Botanical Survey of India, Southern circle, Coimbatore, Tamil Nadu. The collected leaves samples were rinsed with tap water dried and powdered and then stored at 4 °C. Plant extracts preparation 5g of each sample of *R. officinalis* was extracted with 100 ml of methanol using Soxhlet apparatus. The extract was filtered and methanol was evaporated by rotary evaporator and then stored at 4°C for future use.

**Phytochemical Screening**

The methanolic extracts were subjected to chemical tests for the detection of different phytoconstituents using standard procedures.

**Test for Phenols**

To 1 ml of the extract, 3 ml of distilled water followed by few drops of 10%aqeous Ferric chloride solution was added. Formation of blue or green colour indicates the presence of phenols.

**Test for Flavonoids**

To 2 ml of the extract, 1 ml of 1% ammonia solution was added. Appearance of yellow colour indicates the presence of flavonoids.

**Test for Tannins**

To 1 ml of the extract, 1 ml of 0.008 M Potassium ferricyanide was added and then add 1ml of 0.02 M Ferric chloride containing 0.1 N HCl. Appearance of blue-black colour indicates the presence of Tannins.

**Test for Alkaloids**

Approximately, 1 ml of crude extract was mixed with 2 ml of Wagner’s reagent. Reddish brown colour precipitate indicates the presence of alkaloids.

**Test for carbohydrates**

Fehling’s test Equal volume of Fehling A and Fehling B reagents were mixed together and then add 2ml of crude extract in it and gently boiled. A brick red precipitate appeared at the bottom of the test-tube indicates the presence of reducing sugars.

Benedict’s test 1 ml of crude extract was mixed with 2ml of Benedict’s reagent and boiled. A reddish brown precipitate was formed which indicates the presence of the carbohydrates.

**Test for proteins**

Millon’s test 1 ml of crude extract was mixed with 2ml of Millon’s reagent, white precipitate appeared which turned red upon gentle heating that confirmed the presence of protein.

Ninhydrin test 1 ml of crude extract was mixed with 2ml of 0.2% solution of Ninhydrin and boiled. A violet colour precipitate was appeared suggesting the presence of amino acids and proteins.

**Test for Cardiac glycosides (Keller-Kiliani test)**

5 ml of extract was treated with 2 ml of glacial acetic acid containing one drop of ferrichloride solution. This was underlayed with 1 ml of concentrated sulphuric acid. A browning of the interface indicates a deoxy sugar characteristic of cardenolides. A violet ring may appear below the brown ring, while in the acetic acid layer, a greenish ring may form just gradually throughout thin layer.

**Test for Saponins**

2 ml of crude extract was mixed with 5 ml of distilled water in a test tube and it was shaken vigorously. Add some drops of olive oil. The formation of stable foam was taken as an indication for the presence of saponins.

**Test for Coumarin**

10 % Sodium hydroxide was added to the extract and chloroform was added. Formation of yellow color shows the presence of Coumarin.

**Test for Terpenoids (Salkowski test)**

5 ml of extract was mixed with 2 ml of chloroform and 3 ml of concentrated sulphuric acid was carefully added to form a layer. A reddish brown colouration of the inter face was formed which indicates the presence of terpenoids.

**Test for Steroids**

2 ml of acetic anhydride was added to 0.5 ml of crude extract containing 2 ml of sulphuric acid. The colour changed from violet to blue or green in samples indicates the presence of steroids.

**Test for Quinones**

Diluted sodium hydroxide was added to the 1 ml of crude extract. Blue green or red coloration indicates the presence of quinones.

**Test for anthraquinones (Borntragers test)**

0.5 g of each extract was boiled with 10% hydrochloric acid for few minutes in water bath. It was filtered and allowed to cool. Equal volume of CHCl₃ was added to the filtrate. Few drops of 10% ammonia was added to the mixture and heated. Formation of rose – pink color indicates of n-hexane, chloroform, ethyl acetate and methanol of the presence of the anthraquinones.

**Preparation and extraction of sample**

Protocol for preparation of sample was according to the methods previously described, with modifications wrt...
temperature and duration of drying the sample. A 100 g leaf was weighed and dried in an oven at 60°C. Dried sample was ground into powder using Thomas-Willey milling machine and sieved on a wire mesh screen (3 x 3 mm²). Sample was stored at 4°C in air-tight container with screw caps. Sample was prepared according to the methods previously described.25 25 g of sample was suspended in 250 mL of distilled water in stoppered flasks and allowed to stand for 24 h, filtered with Whatman No 24 filter paper, concentrated in a rotary evaporator for 12 h at 50°C and dried in vacuum desiccator and subjected to GC-MS analysis.

**GC-MS Analysis**

Phy-co-components were identified using GCMS detection system as previously with minor modification, Whereby portion of the extract was analysed directly by headspace sampling. GCMS analysis was accomplished using an Agilent 7890A GC system set up with 5975C Vl MSD (Agilent Technologies, CA, and USA). Capillary column used was DB-5MS (30 m × 0.25 mm, film thickness of 0.25 µm; J&W Scientific, CA, USA). Temperature program was set as follows: initial temperature 50°C held for 1 min, 5°C per min to 100°C, 9°C per min to 200°C held for 7.89 min, and the total run time was 30 min. The flow rate of helium as a carrier gas was 0.811851 mL/min. MS system was performed in electron ionization (EI) mode with Selected Ion Monitoring (SIM). The ion source temperature and quadruple temperature were set at 230°C and 150°C, respectively. Identification of phy-co-components was performed by comparison of their retention times and mass with those of authentic standards spectra using computer searches in NIST 08 and Wiley 7nL libraries.

**RESULTS AND DISCUSSION**

**Chemical Properties and Identifier**

- Chemical kingdom: Organic compounds
- Superclass: Lipids and lipid-like molecules
- Class: Prenol lipids
- Subclass: Monoterpenoids
- PubChem Identifier: 170833
- Synonyms: ISOPULEGOL; ALPHA-TERPINOLE; LINALYL ACETATE
- Canonical SMILES: C[@@H][1]C[C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[@@H][1]C[CODEN (USA): JDJTAO

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Table 1 Qualitative phytochemical analysis of methanolic extract of *R. officinalis*

| PHOTOCONSTITUENTS | TEST                      | PRESENT/ ABSENT |
|--------------------|---------------------------|-----------------|
| Phenol             | FeCl3 Test                | +++             |
| Flavonoids         | Shinoda Test              | ++              |
| Tannins            | FeCl3 Test                | ++              |
| Alkaloids          | Wagner’s reagent Test     | +               |
| Carbohydrates      | Fehling’s test, Benedict’s test | ++     |
| Proteins           | Millon’s Test, Ninhydrin Test | ++  |
| Glycosides         | Keller-Kiliani Test       | +               |
| Saponins           | Foam Test                 | +               |
| Coumarins          | Coumarins Test            | +               |
| Terpenoids         | Salkowski Test            | ++              |
| Quinones           | Quinone Test              | +               |
| Steroids           | Salkowski Test            | +               |
| Anthraquinones     | Borntrager’s Test         | -               |

+++ = Copiously present; ++ = moderately present; + = slightly present; - = absent

Figure 1: GCMS analysis of *Rosmarinus officinalis* (Rosemary) essential oil

Table 2: GCMS profile of *Rosmarinus officinalis* (Rosemary) essential oil

| S.No | Compound       | Molecular Formula | Retention Time (min) | Percentage (%) |
|------|----------------|-------------------|----------------------|----------------|
| 1.   | α-Pinene       | C_{10}H_{16}O     | 6.94                 | 13.64          |
| 2.   | Camphene       | C_{10}H_{16}      | 7.38                 | 2.42           |
| 3.   | β-Myrcene      | C_{10}H_{16}      | 8.88                 | 1.19           |
| 4.   | α-Terpinine    | C_{10}H_{16}      | 9.70                 | 0.41           |
| 5.   | p-Cymene       | C_{10}H_{14}      | 9.98                 | 6.23           |
| 6.   | trans-3-Caren-2-ol | C_{10}H_{16}O   | 10.10                | 0.20           |
| 7.   | 1,8-Cineole    | C_{10}H_{18}O     | 10.38                | 41.75          |
| 8.   | γ-Terpinene    | C_{10}H_{16}      | 11.25                | 0.59           |
| 9.   | α-Terpinolene  | C_{10}H_{16}      | 12.30                | 0.35           |
| 10.  | Linalool       | C_{10}H_{18}O     | 12.78                | 1.19           |
|   | Chemical Name       | Molecular Formula | Molecular Properties | Biological Properties |
|---|---------------------|-------------------|----------------------|-----------------------|
| 11. | Isopulegol         | C_{10}H_{16}O     | miLogP 3.65           | GPCR ligand -1.11     |
| 12. | Eucalyptol         | C_{10}H_{18}O     | TPSA 0.00             | Ion channel modulator -0.81     |
| 13. | Terpinen-4-ol      | C_{10}H_{18}O     | natoms 10             | Kinase inhibitor -1.41     |
| 14. | 2-Naphthalenol     | C_{10}H_{18}O     | MW 134.22             | Nuclear receptor ligand -1.23     |
| 15. | (-)-Myrtenol       | C_{10}H_{16}O     | nON 0                 | Protease inhibitor -1.47     |
| 16. | Verbenone          | C_{10}H_{14}O     | nOHNH 0               | Enzyme inhibitor -0.77     |
| 17. | Terpine            | C_{12}H_{20}O_2   | nviolations 0         |                        |
| 18. | α-Copaene          | C_{15}H_{24}      | nrotb 1               |                        |
| 19. | β-Caryophyllene    | C_{15}H_{24}      | volume 150.53         |                        |
| 20. | γ-Cadinene         | C_{15}H_{24}      |                        |                        |
| 21. | Caryophyllene oxide| C_{15}H_{24}O     |                        |                        |

**a)**

![Chemical Structure of p-Cymene](image)

**Molecular Properties**
- **miLogP**: 3.65
- **TPSA**: 0.00
- **natoms**: 10
- **MW**: 134.22
- **nON**: 0
- **nOHNH**: 0
- **nviolations**: 0
- **nrotb**: 1
- **volume**: 150.53

**Bioactivity Scores**
- **GPCR ligand** -1.11
- **Ion channel modulator** -0.81
- **Kinase inhibitor** -1.41
- **Nuclear receptor ligand** -1.23
- **Protease inhibitor** -1.47
- **Enzyme inhibitor** -0.77
b) Terpin
(Cyclohexanemethanol, 4-hydroxy-\(\alpha\),\(\alpha\),4-trimethyl-)

\[
\text{CC1(CCC(C1)C(C)(C)O)O}
\]

| Molecular Properties | Values |
|----------------------|--------|
| \text{miLogP}       | 1.61   |
| \text{TPSA}         | 40.46  |
| n\text{atoms}       | 12     |
| MW                   | 172.27 |
| n\text{ON}          | 2      |
| n\text{OHNH}        | 2      |
| n\text{violations}  | 0      |
| n\text{rotb}        | 1      |
| volume               | 184.55 |

Biological Properties

Bioactivity Scores

- GPCR ligand: -0.39
- Ion channel modulator: 0.35
- Kinase inhibitor: -1.12
- Nuclear receptor ligand: -0.35
- Protease inhibitor: -0.55
- Enzyme inhibitor: -0.02

c) Isopulegol
(Cyclohexanol, 5-methyl-2-(1-methylethenyl)-)

\[
\text{CC1CCC(C(C1)O)C(=C)C}
\]

| Molecular Properties | Values |
|----------------------|--------|
| \text{miLogP}       | 2.65   |
| \text{TPSA}         | 20.23  |
| n\text{atoms}       | 11     |
| MW                   | 154.25 |
| n\text{ON}          | 1      |
| n\text{OHNH}        | 1      |
| n\text{violations}  | 0      |
| n\text{rotb}        | 1      |
| volume               | 171.55 |

Biological Properties

Bioactivity Scores

- GPCR ligand: -0.78
- Ion channel modulator: -0.16
- Kinase inhibitor: -1.59
- Nuclear receptor ligand: -0.22
- Protease inhibitor: -0.71
- Enzyme inhibitor: -0.14
Eucalyptol
(1,8-Cineole; 470-82-6; 1,8-Cineol)

\[
CC1(C2CC(O1)(C(C2)C))C
\]

alpha-Pinene oxide
(3-Oxatricyclo[4.1.1.0(2,4)]octane, 2,7,7-trimethyl-)

\[
CC1(C2CC1C3(C(C2)O3)C)C
\]
f) 2-Naphthalenol, decahydro-(-Naphthalenol, decahydro-)

C1CCC2CC(CCC2C1)O

Figure 2a-f Structure (2D, 3D), molecular biological properties of compounds in *R. officinalis*