INTRODUCTION

Genus Cymbopogon is widely distributed in the tropical and subtropical regions of Africa, Asia, and America. The genus Cymbopogon comprises of more than 144 species, and is well known for its high content of essential oils1-2. Studies have led to the isolation of alkaloids, volatile and non-volatile terpenoids, flavonoids, carotenoids and tannins from every part of Cymbopogon species. Cymbopogon martini (lemongrasses) is native to India and Indochina, but widely cultivated in many places for its aromatic essential oil. Known as Palmarosa, the plant has other names: Indian geranium, ginger grass, rosha, and rosha grass. Besides, therapeutic application, it is commonly used as a condiment and food preservative. PEO contains bioactive molecules, phyto-compounds, endowed with pharmacological activities3. PEO contains geraniol, used as scent and in a number of traditional medicinal. PEO is of commercial importance, being extensively used in perfumes, soaps, cosmetics, toiletry and tobacco products4. PEO has effective insect repellent property when applied to stored grain and beans5, antihelminth against nematodes5, antifungal6,7 and mosquito repellent8 activity. CMEO is used in aromatherapy due to its antimicrobial properties. It is used in Ayurvedic medicine to treat skin problems and relieve nerve pain. Immunomodulatory action of CMEO was evaluated towards production of pro- and anti-inflammatory cytokines (TNF-α and IL-10) by human monocytes in vitro9.

Essential Oils (EOs) a major group of Phytogenic Bio-Active Compounds (PBAC) have been used for variety of purposes. Due to their physicochemical properties and bioactive nature, EOs has been used in aromatherapy, as flavor and fragrances in cosmetics, foods, and more recently as pharmaceuticals, natural preservatives, additives, and biopesticides10,11. EOs are concentrated form of liquid mixtures of volatile compounds of plant origin with unique structural chemistry including terpenoid and non-terpenoid hydrocarbons and their oxygenated derivatives, with natural color, odor and flavor, or “essence” of their source - volatile/ odoriferous oil. EOs are extracted from various plant parts such as leaves, fruit, bark, root, wood, heartwood, gum, balsam, berries, seeds, flowers, twigs, and buds12.

Role of EOs in drug development has been well documented since antiquity nevertheless, they are directly used as therapeutic agents due to fact that they have proven record in traditional indigenous systems of medicine such as Ayurveda, Siddha, Unani and Homeopathy and in modern medicine, EOs contain bioactive compounds of GRAS nature. Furthermore, concern about the negative effect of synthetic chemicals as food additives warrants “GO” products with no or lesser side effects. Therefore, growing interest in natural
extracts as alternatives for synthetic additives is attributed to (a) their synergy with other preservation methods (b) generally regarded as safe, and (c) PBNPs are endowed with antioxidant, antidiabetic, antimutagenic, antitoxicogenic and antibacterial properties. Apart from effective antioxidants of CMEO viz., cyclic diterpene diphenols, carnosic acid and carnosol CMEO contains carnosic acid, epicosmonol, rosmanol, methylcarnosate and isorosmonol however, needs scientific validation.

*Cymbopogon martini* (Palmarosa) has been traced for its origin from the Mediterranean region. It is an aromatic plant, a unique spice commercially available for use as an antioxidant. CMEO extracts have been used in the treatment of diseases, due to its phytotherapeutic potential. On the other hand, it is used in food preservation, PEO could even decrease the use of synthetic antioxidants in foods. EFSA (European Food Safety Authority) recently, reviewed the safety of CMEO extracts and concluded that there are high-intake estimates ranging from 0.09 (elderly) to 0.81 (children) mg/kg per day.

**Cymbopogon martini (PALMAROSA)**

**Botanical Description:** Perennial from a short woody rootstock. Culms tufted, up to 3 m tall, lower nodes often swollen, mealy. Leaf sheaths glabrous; leaf blades lanceolate, usually glaucous below, dark green above, up to 50 × 2–3 cm, glabrous, base cordate, often amplexicaul, apex filiform; ligule 2–4 mm. Spathate panicle narrow, dense, erect, 20–30 cm; spatheollae green becoming reddish, 2–3 mm; spatheollae green becoming reddish, 2–3 cm; racemes 1.5–2 cm; rachis internodes and pedicels ciliate on margins, back sometimes pubescent; pedicel of homogamous pair swollen, barrel-shaped, shiny, fused to internode at base. Sessile spikelet oblong, 3.5–4.5 mm; lower glume flat, deeply grooved below middle, keels winged above middle, vein less or 2-veined between keels; upper lemma 2-lobe bed; awn 1.4–1.8 cm. Pedicelled spikelet 3.5–4 mm. Fl. and fr. Jul.–Oct. This grass is native to India, but is cultivated elsewhere in tropical regions of the world for its essential oils.

In traditional medicine both the plant and its oils are used to treat rheumatism, hair loss, arthritis, lumbago and spasms. The essential oil is a strong fungicide. In laboratory tests it was more effective than several synthetic fungicides against pathogenic fungi and yeasts, including *Aspergillus* spp., *Candida albicans*, *Monilia sitithora* and *Trichophyton tonsurae*. In Ayurvedic medicine - Charak gave the decoction of whole plant in the treatment of abdominal disorders, the liver disorders, jaundice, fever and disorders of the spleen. In Sushruta, decoction of whole plant is prescribed in inflammation of throat, chest pain, indigestion, bronchitis, cough and asthma.

**MATERIALS AND METHODS**

**Collection, Preparation and Extraction of Oil from the sample**

The leaf samples were collected from wild in the Perumalmalai Region (Perumalmalai is a hillock in the Palani Hills, Dindigul District, Tamil Nadu) Western Ghats, INDIA during December 2020. The leaf sample were well preserved, taken to laboratory, identified by using flora and shade dried and processed as per the protocol for preparation of sample according to the methods previously described by Eleyinmi, however, with modifications in the temperature and duration of processing of the sample. As much as 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 × 3 mm²). Sample was stored at 4°C in air-tight container with screw caps. Sample was prepared according to the methods previously described by Raškov et al. 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. Yield was calculated to be 6.06% w/w. Extract was suspended in ethyl acetate and subjected to GC-MS analysis.

**GC-MS Analysis**

*Cymbopogon martini* (Palmarosa) Essential Oil was extracted, from the leaf samples collected from the Perumalmalai Region, Palani, Dindigul District, Tamil Nadu, India. Phyto-components were identified using GC-MS detection system as described previously, however with modification, whereby portion of the extract was analysed directly by headspace sampling. GC-MS 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 quadrupole temperature were set at 230°C and 150°C, respectively. Identification of phyto-components was performed using comparison of their retention times and mass with those of authentic standards spectra using computer searches in NIST 08L and Wiley 7nl libraries.

**ADMET prediction**

Selected phytocompounds were subjected to ADMET prediction using QikProp (version 4.3, Suite 2015-1; Schrödinger, LLC, New York, NY) and toxicity prediction using TOPKAT (Accelrys, Inc., USA). QikProp develops and employs QSAR/QSPR models using partial least squares, principal component analysis and multiple linear regression to predict phisico-chemically significant descriptors.

**RESULTS AND DISCUSSION**

**GCMS analysis**

The chemical composition of EOs depends on plant genetics, growth conditions, development stage at harvest, and processes of extracting active compounds. Different parts of the plant (bark, leaf, fruit and seed) have been extensively investigated for their bioactive phytochemical constituents in various plants. GC-MS analysis revealed that the extract of *Cymbopogon martini* contained different volatile oils (Jummes et al., 2020), 4-Decen-6-yn-1-ol (Z) (C10H18), 3.568 min, 10 hits; 2-Ethylmethyl-4-methyl-pent-3-enenitrile (C10H14N). 3.913 min, 10 hits; Cyanogen bromide (CBrN), 4.024, 1 hits; Cyclohexane, 2-methyl-5-{1-methylthienyl}, (1L-PhaA,2,5a,5b) - (C10H18O). 4.503 min, 10 hits; Cyclohexa-1,3-diene, 5,6-diyethyl- (C10H14). 4.915 min, 10 hits; Benzaldehyde, 2-methyl- (C6H8O). 8.154 min, 10 hits; Pyrazine (C4H4N2), 9.32, 5 hits; 2-Norborenonecatic acid (C10H16O2), 9.378, 8 hits; cis-syn-trans-Tricyclo[7.3.0.0 (2,6)]dodec-7-ene (C10H16), 9.509 min, 10 hits; 12,4-Methano-1-H-indene, octahydr-1,7a-dimethyl -5-{1-methylthienyl}, [1S (1L-PhaA,2a,5b,5a,5aa)a,6a(7.85)] - (C10H18O). 9.913 min, 10 hits; 1,4,7-Cyclo-decatriene, 1,5,9-pentamethyl-1,5,9-(C10H18). 10.343 min, 10 hits; Naphthalene, decabhydro-4a-methyl-1-methylen-7-{1-methylthiolide}, (4aR-trans)- (C10H18). 10.738 min, 10 hits; Butanoic acid, 3,7-dimethyl-2,6-
Biological activities of these secondary metabolites of Cymbopogon martini (Palmarosa) have been reported for its antitumor, antioxidant, anti-inflammatory, and analgesic activities and effects on the central nervous system, endocrine system, disorders such as cardiac and analgesic activities, and effects on the central nervous system, endocrine system, disorders such as cardiac and analgesic activities.

Similarly, ADMET properties of key molecules in CMO (Caryophyllene oxide and Geranyl butyrate) towards Human Intestinal Absorption, Blood Brain Barrier, Caco-2 permeable, P-glycoprotein substrate, P-glycoprotein inhibitor I, P-glycoprotein inhibitor II, CYP450 2C9 substrate, CYP450 2D6 substrate, CYP450 3A4 substrate, CYP450 1A2 inhibitor, CYP450 2D6 inhibitor, CYP450 2C9 inhibitor, CYP450 3A4 inhibitor, CYP450 inhibitory promiscuity, Ames test, Carcinogenicity, Biodegradation, Rat acute toxicity, LD50 mol/kg, hERG inhibition (predictor I), hERG inhibition (predictor II) (Table 5) indicate that these molecules can be used for drug formulations.

### Table 1: GC-MS profile of compounds in C. martini essential oil

| RT       | Name of the Compound                                                | Molecular Formula | Hits (DB) |
|----------|---------------------------------------------------------------------|-------------------|-----------|
| 3.568    | 4-Decen-6-yn, (Z)-                                                 | C₆H₁₆             | 10        |
| 3.913    | 2-Ethylmino-4-methyl-pent-3-enenitrile                              | C₈H₁₂N₂           | 10        |
| 4.024    | Cyanogen bromide                                                   | CBrN              | 1         |
| 4.503    | Cyclohexanol, 2-methyl-5-(1-methylethenyl) (1.alpha.,2.beta,5.alpha.)-| C₁₀H₁₀O          | 10        |
| 4.915    | Cyclohexa-1,3-diene, 5,6-diethyl-                                   | C₆H₁₆             | 10        |
| 8.154    | Benzaldehyde, 2-methyl-                                            | C₆H₁₀             | 10        |
| 9.32     | Pyrazine                                                           | C₄H₈N₂           | 5         |
| 9.378    | 2-Norbornaneacetic acid                                            | C₄H₄O₂           | 8         |
| 9.509    | cis-syn-trans-Tricyclo[7.3.0.(2,6)]dodec-7-ene                      | C₁₂H₁₈           | 10        |
| 9.913    | 1,2,4-Metheno-1H-indene, octahydropenta-1,7a-dimethyl-5-(1-methylethyl), [1S- (1.alpha,2.alpha,3a.beta,4.alpha,5.alpha,7a.be ta,8S*)]-| C₁₃H₂₄          | 10        |
| 10.343   | 1,4,7-Cycloundecatriene, 1,5,9,9-tetramethyl-                        | C₁₃H₂₄           | 10        |
| 10.738   | Naphthalene, decahydro-4a-methyl-1-methylene-7-(1-methylethylidene)-, (4aR-trans)- | C₁₃H₂₄          | 10        |
| 11.772   | Butanoic acid, 3,7-dimethyl-2,6-octadienyl ester,(E)-              | C₈H₁₂O₂          | 10        |
| 11.948   | Nerolidol 2                                                        | C₁₅H₂₀O          | 10        |
| 12.525   | Caryophyllene oxide                                                | C₁₅H₂₀O          | 10        |
| 15.152   | 2-Azidomethyl-1,3,3-trimethyl-cyclohexene                           | C₁₅H₂₀N₃         | 10        |
| 15.423   | Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester,(E)-              | C₁₆H₂₂O₂         | 10        |
| 17.258   | Farnesol, acetate                                                  | C₁₆H₂₂O₂         | 10        |
| 20.158   | 2,6-Octadien-1-ol, 3,7-dimethyl-, propanoate,(Z)-                 | C₁₃H₂₂O₂         | 10        |
Table 2: IUPAC Name, 2D, 3D structure of bioactive compounds in CMEO

| IUPAC Name                                | 2D Chemical Structure | 3D Chemical Structure |
|-------------------------------------------|-----------------------|-----------------------|
| Cyclodecyne; 4-Decen-6-yne, (Z)           | ![Chemical Structure](image1) | ![Chemical Structure](image2) |
| 2-Ethylimino-4-methyl-pent-3-enenitrile   | ![Chemical Structure](image3) | ![Chemical Structure](image4) |
| Dihydrocarvyl acetate                     | ![Chemical Structure](image5) | ![Chemical Structure](image6) |
| 2-Methylbenzaldehyde                      | ![Chemical Structure](image7) | ![Chemical Structure](image8) |
| Geranyl butyrate                          | ![Chemical Structure](image9) | ![Chemical Structure](image10) |
| 1,5,9,9-Tetramethyl-1,4,7-cycloundecatriene | ![Chemical Structure](image11) | ![Chemical Structure](image12) |
| Caryophyllene oxide                       | ![Chemical Structure](image13) | ![Chemical Structure](image14) |

Table 3: Molecular properties of bioactive compounds in CMEO

| PROPERTY      | BIOACTIVE COMPOUNDS |
|---------------|---------------------|
| CID           | 137799  68315  73918  998  5282854  5281522  1742210 |
| MF            | C_{10}H_{16}  C_{10}H_{12}N_{2}  C_{10}H_{16}O  C_{10}H_{16}O  C_{14}H_{24}O_{2}  C_{15}H_{24}  C_{15}H_{24}O |
| miLogP        | 4.54  2.09  3.35  2.13  4.83  5.07  4.14 |
| TPSA          | 0.00  36.16  26.30  17.07  26.30  0.00  12.53 |
| N atoms       | 10  10  4  9  16  15  16 |
| MW (g/mol)    | 136.24  136.20  154.24  120.15  224.34  204.36  220.36 |
| Non           | 0  2  2  1  2  0  1 |
| n OHNH        | 0  0  0  0  0  0  0 |
| N violations  | 0  0  0  0  0  1  0 |
| N rotb        | 3  2  3  1  8  0  0 |
| volume        | 162.53  146.66  208.06  119.59  245.69  234.00  234.01 |
Studies have led to the isolation of alkaloids, volatile and non-volatile terpenoids, flavonoids, carotenoids and tannins from *Cymbopogon* species. β-Caryophyllene from CMOE has been reported to be directly beneficial for colitis, osteoarthritis, diabetes, cerebral ischemia, anxiety and depression, liver fibrosis. Biological activities of these secondary metabolites of *Cymbopogon martini* (Palmarosa) have been reported for its antitumor, antioxidant, anti-infectious, anti-inflammatory, and analgesic activities and effects on the central nervous system, endocrine system, disorders such as cardiac remodeling after myocardial infarction, body weight changes, dyslipidemia, cerebral ischemia, hepato-nephrotoxicity, stress, and anxiety. Anti-inflammatory activity of CMOE has been attributed to the

| PROPERTY | BIOACTIVE COMPOUNDS |
|----------|---------------------|
| CID      | 137799 68315 73918 998 5282854 5281522 1742210 |
| GPCR ligand | -0.56 -1.64 -0.47 -2.33 -0.26 0.03 0.08 |
| Ion channel modulator | 0.57 -1.04 0.23 -1.80 0.05 0.132 0.14 |
| Kinase inhibitor | -1.05 -2.08 -1.25 -2.40 -0.86 -0.95 -0.86 |
| Nuclear receptor ligand | -0.18 -2.06 -0.17 -2.20 0.03 0.40 0.62 |
| Protease inhibitor | 0.43 -0.84 -0.12 -1.91 0.30 0.41 0.57 |

Note: MP = Mutagenic property; TP = Toxicology property; IP = Irritant property; RE = Reproductive property; DL = Drug Likeness; DS = Druggable Score

Table 5: Summary of MTIR/ DL/DS score of bioactive compounds in CMOE

| COMPOUND | MP | TP | IP | RE | DL | DS |
|----------|----|----|----|----|----|----|
| Cyclodecyne; 4-Decen-6-yne,(Z)- | None | None | High | None | -10.80 | 0.21 |
| 2-Ethylmino-4-methyl-pent-3-enenitrile | None | None | None | None | -4.87 | 0.48 |
| Dihydrocarvyl acetate | None | None | High | None | -19.56 | 0.26 |
| 2-Methylbenzaldehyde | None | None | Medium | High | -5.59 | 0.23 |
| Geranyl butyrate | None | None | None | High | -5.84 | 0.21 |
| 1,5,9,9-Tetramethyl-1,4,7-cycloundeacatriene | None | None | None | None | -5.08 | 0.28 |
| Caryophyllene oxide | None | Medium | None | Medium | -4.77 | 0.25 |

Table 6: Druggability Properties of bioactive compounds in CMOE

| Druggability Property | BIOACTIVE COMPOUNDS |
|-----------------------|---------------------|
| Lipinski's rule of 5 violations | 0 0 0 0 0 0 |
| Veber rule | Good Good Good Good Good |
| Egan rule | Good Good Good Good |
| Oral PhysChem score | 0 1 2 2 1 2 |
| GSK's 4/400 score | Good Good Good Good Good |
| Pfizer's 3/75 score | Warning Bad Bad Bad Bad |
| QEDw score | 0.521 0.506 0.493 0.434 0.433 0.434 |
| Solubility | 12379.28 8150.46 4750.64 5166.30 4350.64 5166.30 |
| Solubility Index | Good Good Good Good Good |

Druggability scoring schemes were computed using FAF-Drugs 4(28961788) and FAF-QED 4(28961788) open-source Chem-informatics platform.
presence and synergistic activity of carnosol and carnosic, rosmarinic, ursolic, oleanolic, and micromeric acids (A). Specifically, anti-inflammatory activity has been attributed to synergic effects of ursolic and micromeric acids present in CMEO. These natural drugs can be proposed for preclinical and clinical studies in different diseases and pathological conditions.

CONCLUSION

_Cymbopogon_ species have been used as traditional medicine in many countries since antiquity. CMEO has been used in traditional and in conventional medicine due to the pharmacological potential of their phytochemicals. _C. martini_ (Palmarosa) contains a large variety of bioactive molecules with great therapeutic potential and biological activities such as insecticidal, anti-protozoan, anticancer, anti-HIV, anti-inflammatory and anti-diabetes effects. CMEO has remarkable anti-inflammatory, antimicrobial, and antioxidant properties, which have been extensively reported in several formulations. However, development of new formulations containing other less common CMEO extracts is warranted through trials to establish the credentials of pharmacologically active phyto-compounds towards safety/ efficacy, in treating various pathological conditions including COVID-19 and other viral infections owing to the physicochemical properties and druggable nature of CMEO.

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