Data Article

Data on GC-MS analysis, in vitro anti-oxidant and anti-microbial activity of the *Catharanthus roseus* and *Moringa oleifera* leaf extracts

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**Abstract**

The article reports data on chemical profiling by gas chromatography-mass spectrometry (GC-MS) of aqueous and methanolic leaf extracts of Madagascar periwinkle (*Catharanthus roseus*) and drumstick tree (*Moringa oleifera*) and on their anti-oxidant and antibacterial effects against three clinical human pathogens. In total 105 compounds were tentatively identified; in which 65 in *Catharanthus roseus* and 40 in *Moringa oleifera* compounds. A large number of peaks with good area percentage was found in methanolic extract of *Catharanthus roseus* with core chemical constituents such as trans-squalene, n-hexadecanoic acid, Eicosyl acetate, stearin, 1H-Benz(G)indole-3-carboxylic acid. The corresponding constituents from *Moringa oleifera* include 9-Octadecenoic acid (z)-, Heptadecanoic acid and phytol acetate. The highest scavenging activity (87.7% at 200 µg/mL) was shown by DPPH aqueous leaf extract of *C. roseus*. Moreover, the methanolic scavenging of both plant extracts was in the order of FRAP>DPPH>NO> H₂O₂ with lowest antioxidant activity (51.4% at 200 µg/mL) exposed by *Catharanthus roseus* in comparison of all cases. Good antibacterial action was examined against three different organisms (*E.coli, B. subtilis* and *S. aureus*) of aqueous infusion of *Catharanthus roseus*.

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1. Data

The current data pertains to GC—MS chromatogram of the methanolic and aqueous leaf extract of C. roseus (Figs. 1 and 2) and M. oleifera (Figs. 3 and 4) with their corresponding secondary metabolites as depicted in Tables 1 and 2 respectively. In-vitro antioxidant assays with percentage of inhibition as a parameter are presented in Figs. 5 and 6. Antimicrobial activity (in terms of inhibition zones) of C. roseus and M. oleifera leaves against selected bacterial strains was shown in Table 3.

2. Experimental design, materials and methods

2.1. Collection of plant material and preparation

The fresh leaves of Catharanthus roseus (Apocynaceae) and Moringa oleifera (Moringaceae) were gathered from campus of Yogi Vemana University, Kadapa and near Raychotighat, India respectively. The plant specimens were recognized and authenticated by Department of Botany at Yogi Vemana University, Kadapa, India. The leaves of both the plants were harvested at the vegetative phase.
2.2. Plant sample extraction and column chromatography

Dried powdered leaf samples were successively extracted by soxhlet apparatus, as described by Sadasivam and Manickam [1] and extracts were subjected to column chromatography over silica gel (60–120 mesh) and eluted with n-hexane, chloroform and methanol respectively. n-hexane and chloroform did not elute much of the compounds. Both aqueous and methanolic fractions of *Catharanthus roseus* and *Moringa oleifera* were kept under vacuum desiccators until used for gas chromatography/mass spectrometry (GC–MS) analysis.

2.3. Gas chromatography/mass spectroscopy (GC/MS) analysis

The GC-MS analysis was conducted on GC-MS QP2010 Plus (Shimadzu, Japan) equipped with a flame ionization detector and GC 6890 model series. The GC was equipped with a fused silica
(30 m × 0.25 mm ID × 0.25 μm) capillary column. Injection temperature was maintained at 250 °C by employing helium (99.995%) as a carrier gas at a constant flow rate of 1.5 ml/min. 1 mg/1 ml absolute alcohol at a split ratio of 1:10 was injected. The instrument was set to an initial temperature of 50 °C for 2 min. At the end of this period the oven temperature was arisen up to 300 °C, at the rate of 12 °C/40 min. The mass spectra of compounds in samples were obtained by electron ionization (EI) at 70 eV, and the data was evaluated using total ion count (TIC) for compound identification and quantification. The MS start and end time (3 and 32 min.) was performed at a scan speed of 2000. The spectrum of the
Table 1
Phytochemicals tentatively identified based on retention time (RT) matching in the methanolic (Left) and aqueous (Right) extracts of *Catharanthus roseus* leaf extract by GC-MS.

| Sl. No | RT (min.) (Methanolic) | NIST DATABASE/Wiley 2007/FAME ID/ (Methanolic) | RT (min.) (Aqueous) | NIST DATABASE/Wiley 2007/FAME ID/ (Aqueous) |
|--------|------------------------|-----------------------------------------------|---------------------|-----------------------------------------------|
| 1      | 3.34                   | 2-Hydroxy-2-methyl-4-pentanone (diacetone)     | 6.46                | R (-)-2-Amino-1-butanol                       |
| 2      | 8.23                   | 4-Penten-2-Ol, 3-methyl-                        | 6.55                | Phenethylamine, alpha-ethyl-                  |
| 3      | 14.17                  | Quinoline, 1,2-dihydro-2,2,4-trimethyl-         | 6.77                | 1-Butanol, 2-amino-                          |
| 4      | 15.85                  | Hexathiane                                      | 7.67                | 2,4(1H,3H)-Pyrimidinedione                    |
| 5      | 17.75                  | Pentadecane                                     | 8.23                | Naphthalene                                   |
| 6      | 19.20                  | 2(3H)-Benzothiazolone                           | 8.42                | 2,2,5,5-Tetramethylhex-3-ene, 3,4-dideuterio  |
| 7      | 19.94                  | Octadecane                                      | 8.67                | 4-Pyrimidinamine, 2,6-dimethyl                |
| 8      | 21.16                  | Tetradecanoic Acid                              | 15.09               | Phenol, 2,4-Bis(1,1-dimethylthyl)              |
| 9      | 22.07                  | Tetracosane                                     | 18.20               | Cyclooctasiloxane, hexadecamethyl             |
| 10     | 22.32                  | Octadecanoic Acid                               | 20.29               | 1.3-Diphenyl-1,3,5,5-tetramethyl-             |
| 11     | 23.63                  | 3-(2-Chloroethyl)-1,3-benzothiazol-2(3H)-one    | 20.72               | 1,1,3,5,5,7,9,9,11,11,13,13-Tetradeca         |
| 12     | 24.10                  | Tetracosane                                     | 21.68               | Phosphine Oxide, bis(Pentamethylphenyl)-      |
| 13     | 24.75                  | 2-(1,3-Benzothiazol-2-ylsulfanyl)ethanol        | 22.14               | Hexadecanoic Acid, methyl ester               |
| 14     | 25.25                  | n-Hexadecanoic acid                             | 22.64               | n-Hexadecanoic Acid                           |
| 15     | 25.66                  | Tetracosane                                     | 24.15               | 9-Octadecanoic acid, Methyl ester, (E)-       |
| 16     | 26.78                  | Decane, 1,1'-oxybis-                           | 24.27               | Cyclodecasiloxane, tetracosamethyl            |
| 17     | 27.05                  | Octahexancane                                   | 24.39               | Hexacosiloxane, Methyl Ester                  |
| 18     | 27.93                  | Tetracosane                                     | 24.61               | 1,5,9,9-Tetramethyl-2-oxatricyclo[6.4.0.0(4.8)] |
| 19     | 28.68                  | Urea                                            | 24.98               | 2-Furanapentoic acid, tetrahydro-5-nonyl-, methyl |
| 20     | 29.72                  | Spiro [Cyclopentane-1,2' (1'h)-quinoxaline], 3'- (4-morpholinyl)-6',8'-dinitro- |
| 21     | 29.63                  | Eicosyl Acetate                                 | 25.74               | Cyclononasiloxane, Octadecamethyl-           |
| 22     | 31.44                  | Tetracosane                                     | 27.42               | 1H-Purin-6-Amine, [(2-fluorophenyl)            |
| 23     | 32.55                  | Stannane, Tributyl (2,5-dimethyl-1-phenyl-4- hexenyl)-, (R*R*)*(+--+)-- |
| 24     | 32.74                  | Methyl 6,7-dideoxy-6-C-methyl-2,3-di-octyl- alpha-D-gluco-oct-6-eno-1,5-pyranosid)Urono-8,4-lactone |
| 25     | 33.21                  | Hexadecanoic acid, 2-hydroxy-1- (hydroxymethyl)ethyl ester |
| 26     | 34.78                  | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester |
| 27     | 34.91                  | 1,4-Cyclooctadecane                             | 30.01               | 1,2-Benzenedicarboxylic acid                  |
| 28     | 35.42                  | 1,2-Benzenedicarboxylic acid                    | 32.52               | Cyclononasiloxane, octadecamethyl-           |
| 29     | 35.51                  | Pyrrolo [3,4-C]pyrrole-1-carboxylic Acid, 3- cyclopropylloctahydro-4,6-dioxo-1,5-diphenyl-, methyl ester |
| 30     | 36.93                  | 4,4'((phenylene)diisopropylidene)diphenol       | 37.31               | 1H-indole-3-ethanamine                        |
| 31     | 37.90                  | Octadecanoic acid, 2,3-dihydroxypropyl ester    | 38.40               | Heptacyclo [6.6.0.0(2,6),0(3,13),0(4,11),0(5,9),0(10,14)] |
| 32     | 38.40                  | Heptacyclo [6.6.0.0(2,6),0(3,13),0(4,11),0(5,9),0(10,14)] |
| 33     | 39.28                  | Tetradecane                                     | 40.12               | 1H-Benz [G]indole-3-carboxylic acid, 1-(2,2- dimethoxyethyl)-5-methoxy-2-methyl-, ethyl Ester |
| 34     | 40.59                  | 1H-Benz [G]indole-3-carboxylic acid, 1-(2,2- dimethoxyethyl)-5-methoxy-2-methyl-, ethyl Ester |
| 35     | 41.09                  | Cholest-5-en-3-ol (3.Beta)-                    | 43.30               | 6-Methoxy-2,8-dimethyl-(4',8'-dimethyl-3',7'- nonadienyl)-3,4-dihydro-2H-1-Benzopyran        |
| 36     | 43.89                  | 6-Methoxy-2,8-dimethyl-(4',8'-dimethyl-3',7'- nonadienyl)-3,4-dihydro-2H-1-Benzopyran        |
| 37     | 45.74                  | Beta-Sitosterol                                  | 45.93               | 3-Butoxy-1,1,1,5,5,5-hexamethyl-3- (Trimethylsiloxy)trisiloxane |
| 38     | 45.92                  | Ethanol, 1,1'-[3,3'-bisoxazole]-5,5'-diylbis-   |
| 39     | 46.92                  | 3-Butoxy-1,1,1,5,5,5-hexamethyl-3- (Trimethylsiloxy)trisiloxane |
unknown components were compared with spectrum of known components stored both in the “NIST-MS Library 05”, “Wiley GC-MS Library 2007” as well as FAME with more patterns.

2.4. In-vitro anti-oxidant assays

2.4.1. DPPH free radical scavenging assay

The DPPH radical-scavenging activity of the test extracts was examined using the modified method by Brand-Williams et al. [2]. Leaf extracts of different concentrations (50–200 μg/mL) were mixed with an equal volume of methanolic solution of DPPH (Sigma Aldrich). The mixture was allowed to react at room temperature in dark for 30 min. Ascorbic acid (1 mg/mL (50–200 μg/mL)) was used as positive control. After 30 min the absorbance was measured at 517 nm and converted into percentage of antioxidant activity using the following equation.

\[
\text{% of inhibition} = \left( \frac{A_0-A_1}{A_0} \right) \times 100
\]

\[A_0 = \text{Absorbance of control.}\]
\[A_1 = \text{Absorbance of test.}\]

2.4.2. Hydrogen peroxide scavenging assay

The \( \text{H}_2\text{O}_2 \) scavenging activities for both the leaf extracts were assayed by the modified method [3]. Different concentrations of plant leaf extracts (50–200 μg/mL) and ascorbic acid at different concentrations (50–200 μg/mL) of (1 mg/mL) were added to 40 mM \( \text{H}_2\text{O}_2 \) solution prepared in phosphate buffer. The absorbance of \( \text{H}_2\text{O}_2 \) at 230 nm was determined after 10 min. The percentage of \( \text{H}_2\text{O}_2 \) scavenging by the extracts and standard \( \text{H}_2\text{O}_2 \) was calculated as follows.

\[
\text{% of scavenged [H}_2\text{O}_2] = \left( \frac{A_0-A_1}{A_0} \right) \times 100
\]

\[A_0 = \text{Absorbance of control.}\]

### Table 2

Phytochemicals tentatively identified based on retention time (RT) matching in the methanolic (Left) and aqueous (Right) extracts of *Moringa oleifera* leaf extract by GC-MS.

| Sl. No | RT (min.) (Methanolic) | NIST DATABASE/Wiley 2007/ FAME ID/ | RT (min.) (Aqueous) | NIST DATABASE/Wiley 2007/ FAME ID/ |
|--------|------------------------|----------------------------------|---------------------|----------------------------------|
| 1.     | 8.718                  | 1,1-Diethoxy-2-ethylhexane        | 17.640              | Benzene, 1,1′-(1,2-cyclobutanediyl |
| 2.     | 9.878                  | Azulene                          | 18.252              | 3,7,11,15-Tetramethyl-2-hexadecen-1-ol |
| 3.     | 13.948                 | 2,6-Di-butyl-2,5-cyclohexadiene-1 | 18.736              | Pentadecanal- |
| 4.     | 17.719                 | 9-Octadecenoic acid, ethyl ester  | 19.645              | 9-Octadecenoic acid (z)- |
| 5.     | 17.896                 | 2(4H)-Benzo[1,2-c:3,4-c']dithiophene | 19.742         | 1,2-Benzenedicarboxylic acid, diheptyl ester |
| 6.     | 18.249                 | 2,6,10-Trimethyl,14-ethyleno-14-pe| 19.925              | 2,5-Pyrrolinedione, 1-hydroxy- |
| 7.     | 18.343                 | 2-Pentadecanone, 6,10,14-trimethyl-| 20.085              | Cyclopropanetetradecanoic acid, 2-octyl-, methyl |
| 8.     | 18.519                 | 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | 20.857         | Phosphonic acid, dioctadecyl ester |
| 9.     | 18.736                 | Phthalic acid, isobutyl unde-2-en-1-yl ester | 21.842             | Dimethylaminato [4-methyl-2-(e) |
| 10.    | 19.587                 | 1-[(+)-Ascorbicacid2,6-dihexadecanoate | 22.122              | Tetradecanamide |
| 11.    | 19.750                 | Dibutyl phthalate                | 24.740              | Heptadecanoic acid, ethyl ester |
| 12.    | 19.882                 | Hexadecanoic acid, ethyl ester   | 25.224              | Hexanedioic acid, mono (2-ethylhexyl)ester |
| 13.    | 20.846                 | Behenic alcohol                  | 25.544              | Tetracosenyl acetate |
| 14.    | 21.197                 | 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl- | 26.651             | borneol, Pentamethyldisilanyl ether |
| 15.    | 21.550                 | 9,12-Octadecadienoic acid (z,z)- | 26.941              | 7-Propyl-1,3,5-cycloheptatriene |
| 16.    | 21.735                 | (r)-(−)-14-Methyl-8-hexadecen-1-ol| 27.325              | Octane, 1,1′-oxybis- |
| 17.    | 21.827                 | 9,12,15-Octadecatrienoic acid, (z,z,z)- | 28.782             | Bis(2-ethylhexyl) phthalate |
| 18.    | 22.031                 | Heptadecanoic acid, ethyl ester  | 29.462              | (2,3-Diphenylcycloproul methyl phenyl sulfoxide, |
| 19.    | 22.375                 | Phytol, acetate                  | 29.800              | 1,2-Diphenyl-1-isocoumarone |
| 20.    | 28.779                 | Bis(2-ethylhexyl) phthalate      | 30.285              | 7-(Isobut-1-yl)cyclohepta-1,3,5-tr |

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2.4.3. Nitric oxide radical scavenging assay

The nitric oxide (NO) scavenging activity was determined using the method described by Parul et al. [4]. 10 mM sodium nitroprusside was incubated with 100 μL leaf extract for 60 min at 30 °C. After incubation, 100 μL of griess reagent was added. The absorbance of the chromatophore formed during the diazotization of nitrite with sulphanilamide and subsequent coupling with naphthylehylendiamine was measured at 562 nm. Ascorbic acid (1 mg/mL) was at the same concentration was taken as standard.

\[
\% \text{ NO scavenged} = \left( \frac{A_0 - A_1}{A_0} \right) \times 100
\]

where \(A_0\) = Absorbance of control.
\(A_1\) = Absorbance of test.
2.4.4. Ferric reducing power (FRAP) assay

The reducing power was determined by Benzie and Strain [5] with slight modifications. Various concentrations of plant leaf extracts (50–200 µg/mL) were mixed with phosphate buffer and 2 mM potassium ferricyanide. The mixture was incubated at 50 °C for 20 min. TCA was added to the mixture which was then centrifuged at 3000 rpm for 10 min. The upper layer of solution was mixed with distilled water and freshly prepared FeCl₃ solution (0.5 mL) and the absorbance was recorded at 700 nm.
using UV-Visible spectrophotometer (Thermo scientific evolution -201 series). Ascorbic acid (50–200 µg/mL) was used as positive control. Reducing capacity was calculated as follows:

\[
\text{% increase in reducing power} = \left[ \frac{A_{\text{test}}}{A_{\text{blank}}} - 1 \right] \times 100
\]

Where \( A_{\text{test}} \) = Absorbance of test solution.
\( A_{\text{blank}} \) = Absorbance of blank.

2.5. Antimicrobial assay

2.5.1. Test microorganism

One Gram negative *Escherichia coli* (MTCC 443) and two Gram positive *Bacillus subtilis* (MTCC 441), *Staphylococcus aureus* (ATCC 259323) were used as bacterial test organism. The bacterial strains were cultured overnight at 37 °C in Luria-Bertani (LB) medium.

2.5.2. Agar well diffusion method

Antibacterial activities of two plants extract (*Catharanthus roseus* and *Moringa oleifera*) was determined using Agar well diffusion method [6]. The bacterial suspensions containing \( 7 \times 10^5 \) cells/mL were incubated overnight and used for inoculation. 20 ml of molten nutrient agar was poured into the Petri dishes and cooled. All the bacterial suspension was swapped over the medium and 3 wells of 0.5 cm deep were made by using a sterile tip. Each 50 µL of aqueous, methanolic leaf extracts were added to respective wells one with tetracycline (1 µg/mL, Sigma) was added as positive control and other with distilled water as negative control. Tetracycline (antibiotic) was used as positive control. The antimicrobial behavior was determined by measuring Zone of inhibition around the holes in diameter (mm) after incubation.

2.6. Statistical analysis

All assays were performed in triplicate. Mean and standard deviation (SD) was examined for all assays. The results were expressed as mean ± SEM of three experiments. One way ANOVA with Dunnett’s test was followed to compare each concentration with positive control to analyze level of statistical significance. P < 0.05 were considered statistically significant using Graph pad PRISM v.8.0.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.dib.2020.105258.

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