SwissADME predictions of pharmacokinetics and drug-likeness properties of small molecules present in *Spirulina platensis*

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Abstract. *Spirulina platensis* is a microalga that is easy to cultivate. *Spirulina platensis* contains high antioxidants sourced from chemical compounds. Antioxidants can protect against oxidative stress and degenerative diseases. This study aimed to evaluate the chemical profiles of *S. platensis* using Gas Chromatography-Mass Spectrometry (GC-MS) and predict its biological activity using computational analysis (Absorption, Distribution, Metabolism, Excretion) using SwissADME. The GC-MS analysis of *S. platensis* extracts yielded twenty-four compounds. *Spirulina platensis* extracts contain twelve compounds with percentage more than 1%, namely Dodecanoic acid, ethyl ester (27.71%); Ethyl linoleate (19.47%); Octadecenamide (10.99%); Octadecane (9.02%); Methyl gamma-linolenate (8.04%); 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl- [R-[R*,R*- (E)]- (6.92%); Neophytadiene (3.21%); Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (2.68%); Ethyl 9-hexadecenamide (2.05%); 9-Octadecenoic acid (Z)- (1.47%); 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (1.44%); 9-Octadecenamide (1.15%); and 2-Hexadecene, 3,7,11,15-Tetramethyl-2-hexadecene-1-ol (1%). The dominant compound was dodecanoic acid, ethyl ester. The potential biological activity of dodecanoic acid, ethyl ester, is antimicrobial, antioxidant, anti-cancer, anti-candida, mycelial growth inhibition. All compounds in the extract of *S platensis* met the druglikeness according to Lipinski's rules using SwissADME. SwissADME emerged to be simple, robust and accurate method to understand the ADME properties of the compounds present in *Spirulina platensis* phytoconstituents. The ADME analysis results indicated that *S. platensis* extracts could be developed as traditional medicine and nutraceutical products.
1. Introduction

*Spirulina platensis* is bluish-green microalgae or spiral-shaped blue, green algae. *S. platensis* belongs to the Cyanobacteria group, which is capable of photosynthesis and is easy to cultivate. *Spirulina* is a filamentous and single-celled alga of the cyanobacterium species [1]. This algae usually grows in alkaline waters or alkaline conditions. Further research in [2] explained that *S. platensis* could grow well in liquid media with alkaline conditions. *S. platensis* is a microalga that spreads widely in nature and can be found in various types of environments, both in brackish, marine, and freshwaters [3]. In Indonesia, this alga is cultivated in semi-desert areas almost all year round.

*S. platensis* contains many nutritional components and bioactive compounds that can be used as food, cosmetic, and healthy ingredients. *S. platensis* contains carotenoid and chlorophyll bioactive compounds [4], which act as natural ingredients that can be used for functional foods such as ice cream and soft cheese along with yogurt [5]. Several studies have been conducted showing that *S. platensis* contains biological activities that function as disease prevention, such as preventing viral replication, preventing anemia, preventing diseases caused by fatty liver, lowering blood glucose levels, lipid profiles, and lowering blood pressure [6]. *S. platensis* can be antioxidant, anti-inflammatory, and increases endurance [7]. In addition, Spirulina platensis or its extracts show therapeutic properties as the ability to prevent cancer, lower blood cholesterol levels, reduce nephrotoxicity of drugs and toxic metals that protect against harmful radiation effects [3][8][9][10]. *S. platensis* has antimicrobial activity on pathogenic bacteria such as *E. coli* as gram-negative and *S. aureus* as gram-positive bacteria [11][12].

Bioactive compounds with potential as antioxidants in *S. platensis* are orange pigment carotenoids, green pigment chlorophyll, and blue pigment phycocyanin. These bioactive compounds can be used as a supplement to prevent free radicals. Free radicals in the body can damage cells and lead to severe diseases. The content of beta carotene in *S. platensis* is ten times higher than that of carrots. *S. platensis* has the potential as a natural antioxidant capable of donating hydrogen atoms to free radicals such as phenolic compounds, carotenoids, and chlorophyll. Bioactive compounds contained in *S. platensis*, such as beta carotene, are carotenoids [13].

In-silico studies and bioinformatics are releasing a considerable role in the design, screening, and discovery of drugs with a fast time and low cost [14][15][16][17][18]. At present, computer-assisted computations of ADME (Absorption, Distribution, Metabolism, and Excretion) of drugs are being considered for applying an anticipatory and reliable complement of data to experimental accessions. This computational model predicts the pharmacokinetic, physicochemical, and drug properties of small molecules for drugs [19]. SwissADME is a new and far-reaching website run by the Swiss Institute of Bioinformatics (SIB), which promotes bioinformatics services and resources for scientists worldwide [20]. This study aimed to evaluate the chemical profiles of *S. platensis* using Gas Chromatography-Mass Spectrometry (GC-MS) and predict its biological activity using computational analysis (Absorption, Distribution, Metabolism, and Excretion -ADME).

2. Materials and methods

2.1. Materials

Microalgae *S. platensis* powder sample was extracted by maceration method (immersion) using a ratio of 1:10, namely one part of *S. platensis* microalgae powder sample was immersed in ten parts 96% ethanol solution. Maceration was carried out for two days at room temperature in a wide-mouthed glass container and stirred every 24 hours. The solution results in the immersion process were filtered using Whatman filter paper to produce a liquid *S. platensis* extract. The liquid extract was evaporated using a rotary evaporator at a temperature of 80 °C for 80 minutes to obtain a more concentrated extract [21].

2.2. Chemical profile screening with GC-MS
The chemical profile of the S Platensis extract was screened using Gas Chromatography-Mass Spectrometry-GCMS (Hewlett-Packard 6890), with an Agilent 19091S-433 HP-5MS column having a length of 30 m and a diameter of 250 m. A total of 1 L of S Platensis extract (dissolved with methanol) was injected into the GC-MS. The GC column oven temperature is programmed from 700°C to 3000°C. The initial temperature was 700°C (2 min holding time) and rose to 3000°C (7 min holding time) at a speed of 100°C/min. The total run time is 32.0 min. Helium with a purity of 99.9995% was used as the carrier gas at a constant flow of 1.51 ml/min. The GC-MS interface temperature is at 2800°C. The injector and detector temperatures are set at 200°C. 1 μl of the sample was injected in a 1:10 split ratio. MS scanning range is set from 40-1000 Da [22]. Identification of the compound was obtained by comparing the retention time with the original compound with spectral data obtained from the appropriate compound data library. The number of compounds is represented as a percentage of the relative area originating from the integrator [23]. The chemical structure profile screening was based on analysis of the mass spectrum fragmentation pattern compared with the mass spectrum in the National Institute of Standards and Technology (NIST) and Wiley compound profile databases [24].

2.3. Computational analysis (ADME)
The first step is to access the PubChem server (https://pubchem.ncbi.nlm.nih.gov/) to get canonical SMILE information [25]. The second stage is to estimate their ADMET (absorption, distribution, metabolism, and excretion) through SwissADME (http://www.swissadme.ch/) [26][27].

3. Results and discussion

3.1. Results
The results of GC-MS analysis of Spirulina platensis phytoconstituents (Table 1).

| No | R. Time | Formula | Compounds | Area % |
|----|---------|---------|-----------|--------|
| 1 | 12.270  | C_{32}H_{66} | Dotriacontane | 0.50   |
| 2 | 12.980  | C_{11}H_{16}O_{2} | 2(4H)-Benzofuranone, 5,6,7a-tetrahydro-4,4,7a-trimethyl | 0.62   |
| 3 | 13.540  | C_{15}H_{32} | Pentadecane | 0.27   |
| 4 | 14.790  | C_{18}H_{38} | Octadecane | 9.02   |
| 5 | 15.835  | C_{12}H_{25}O_{2} | Propionic acid, 3-(2-Methylcyclohexyl), ethylester | 0.23   |
| 6 | 16.345  | C_{18}H_{36} | Neophytiadiene | 3.21   |
| 7 | 16.405  | C_{20}H_{40} | 2-Hexadecene, 3,7,11,15-tetramethyl, [R-[R*,R*-E]]- | 0.79   |
| 8 | 16.600  | C_{20}H_{44}O | 3,7,11,15-Tetramethyl-2-hexadecen-1-ol | 1.44   |
| 9 | 17.260  | C_{17}H_{30}O | Hexadecanoic acid, methyl ester | 0.21   |
| 10| 17.780  | C_{18}H_{36}O_{2} | Ethyl 9-hexadecenoate | 2.05   |
| 11| 18.015  | C_{14}H_{26}O | Dodecanoic acid, ethyl ester | 27.71  |
| 12| 19.245  | C_{20}H_{44}O | 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-E]]- | 6.92   |
| 13| 19.525  | C_{19}H_{33}O_{2} | Methyl gamma-linolenate | 8.04   |
| 14| 19.695  | C_{20}H_{33}O | Ethyl linoleate | 19.47  |
| 15| 19.820  | C_{18}H_{30}O | 9-Octadecenoic acid (Z)- | 1.47   |
| 16| 19.940  | C_{20}H_{40}O_{2} | Octadecanoic acid, ethyl ester | 0.91   |
| 17| 20.025  | C_{16}H_{33}NO | Hexadecanamide | 0.73   |
| 18| 20.900  | C_{3}H_{5}NO_{5} | Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester | 0.45   |
| 19| 22.590  | C_{16}H_{33}N | Hexadecenenitrile | 0.57   |
| 20| 22.775  | C_{19}H_{36}O_{4} | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | 2.68   |
| 21| 23.265  | C_{18}H_{33}NO | 9-Octadecenamide | 1.15   |
| 22| 24.200  | C_{19}H_{33}O_{2} | 7,10-Octadecadienoic acid, methyl ester | 0.39   |
Next, *Spirulina platensis* chemical profiles are searched for canonical smiles on PubChem web (Table 2).

**Table 2.** The canonical SMILES of the phytoconstituents of *S. platensis*.

| No | Compounds                                                                 | Canonical SMILES                                      |
|----|---------------------------------------------------------------------------|-------------------------------------------------------|
| 1  | Dotriacontane                                                             | CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC|
| 2  | 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl                 | CC1(CCCC2(C1=CC(=O)O2)C)C                              |
| 3  | Pentadecane                                                               | CCCCCCCCCCCCCCCCC                                                                 |
| 4  | Octadecane                                                                | CCCCCCCCCCCCCCCCCCCCCCCC                                                                 |
| 5  | Propionic acid, 3-(2-Methylcyclohexyl)-, ethylester                       | C=CCCCCCCCCCCCCCC(=O)O                                                                 |
| 6  | Neophytadiene                                                             | CC(C)CCCC(C)CCCC(C)CCCC(=C)=C                                                                 |
| 7  | 2-Hexadecane, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-,                  | CC=C(C)CCCC(C)CCCC(C)CCCC(=C)C                                                                 |
| 8  | 3,7,11,15-Tetramethyl-2-hexadecen-1-ol                                    | CCCCCCCCCCCCCCCCCCCC(=C)=CCOC                                                                 |
| 9  | Hexadecanoic acid, methyl ester                                          | CCCCCCCCCCCCCCCCCCCC(=O)OC                                                                 |
| 10 | Ethyl 9-hexadecenoate                                                     | CCCCCCCCCCCCCCCCCCCC(=O)OCC                                                                 |
| 11 | Dodecanoic acid, ethyl ester                                             | CCCCCCCCCCCCCCCCCCCC(=O)OC                                                                 |
| 12 | 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-              | CCCCCCCCCCCCCCCCCCCC(=C)=CCOC                                                                 |
| 13 | Methyl gamma,-linolenoate                                                | CCCCCCCCCCCCCCCCCCCC(=O)OC                                                                 |
| 14 | Ethyl linoleate                                                           | CCCCCCCCCCCCCCCCCCCC(=O)OCC                                                                 |
| 15 | 9-Octadecenoic acid (Z)-                                                 | CCCCCCCCCCCCCCCCCCCC(=O)N                                                                 |
| 16 | Octadecanoic acid, ethyl ester                                           | CCCCCCCCCCCCCCCCCCCC(=O)OCC                                                                 |
| 17 | Hexadecanamide                                                           | CCCCCCCCCCCCCCCCCCCC(=O)N                                                                 |
| 18 | Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester                       | CCCCCCCCCCCCCCCCCCCC(=O)OCC                                                                 |
| 19 | Hexadecenitrile                                                          | CCCCCCCCCCCCCCCCCCCC(=O)N                                                                 |
| 20 | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester               | CCCCCCCCCCCCCCCCCCCC(=O)OC                                               |
| 21 | 9-Octadecanamide                                                         | CCCCCCCCCCCCCCCCCCCC(=O)N                                                                 |
| 22 | 7,10-Octodecadienoic acid, methyl ester                                  | CCCCCCCCCCCCCCCCCCCC(=O)OCC                                                                 |
| 23 | Octadecanamide                                                           | CCCCCCCCCCCCCCCCCCCC(=O)N                                                                 |
| 24 | N-Tetradecanoic acid amide                                               | O=C(N)CCCCCCCCCCCCCCCCCCC                                                                 |

Then observed the physicochemical properties of the phytoconstituents of *S. platensis* (Table 3).

**Table 3.** Physicochemical properties of the phytoconstituents of *S. platensis*.

| Compounds                                                                 | MW    | HA | AHA | RB | HBA | HBD | MR  | TPSA |
|---------------------------------------------------------------------------|-------|----|-----|----|-----|-----|-----|------|
| Dotriacontane                                                             | 450.87| 32 | 0   | 29 | 0   | 0   | 155.94 | 0.00  |
| 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl                 | 180.24| 13 | 0   | 0  | 0   | 0   | 51.35 | 26.30 |
| Pentadecane                                                               | 212.41| 15 | 0   | 12 | 0   | 0   | 74.22 | 0.00  |
| Octadecane                                                                | 254.49| 18 | 0   | 15 | 0   | 0   | 88.64 | 0.00  |
| Propionic acid, 3-(2-Methylcyclohexyl)-, ethylester                       | 198.30| 14 | 0   | 10 | 2   | 1   | 61.10 | 37.30 |
| Compounds | iLOGP | XLOGP3 | WLOGP | MLOGP | SILICOS-IT | Consensus LogP |
|-----------|-------|--------|-------|-------|------------|----------------|
| Dotriacontane | 8.40  | 16.95  | 12.73 | 9.82  | 13.30      | 12.24          |
| 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl | 2.29  | 2.16   | 2.44  | 2.37  | 2.77       | 2.41           |
| Pentadecane | 4.50  | 7.74   | 6.10  | 6.19  | 5.77       | 6.06           |
| Octadecane | 5.23  | 9.37   | 7.27  | 6.92  | 7.10       | 1.18           |
| Propionic acid, 3-(2-Methylcyclohexyl)-, ethylester | 2.74  | 4.40   | 3.77  | 3.04  | 3.49       | 3.49           |
| Neophytadiene | 5.05  | 9.62   | 7.17  | 6.21  | 7.30       | 7.07           |
| 2-Hexadecene, 3,7,11,15-tetramethyl-[R-[R*,R*-(E)]]-3,7,11,15-Tetramethyl-2-hexadecen-1-ol | 5.24  | 9.44   | 7.39  | 7.23  | 7.14       | 7.29           |
| Neophytadiene | 4.71  | 3.89   | 6.36  | 5.25  | 6.57       | 6.22           |
| Hexadecanoic acid, | 4.41  | 7.38   | 5.64  | 4.44  | 5.84       | 5.54           |

MW - molecular weight (g/mol); HA – number heavy atoms; AHA – number aromatic heavy atoms; RB – number rotatable bonds; HBA – number hydrogen bond acceptor; HBD – number hydrogen bond donor; MR - molar refractivity (m³/mol); TPSA - topology polar surface area (Å²)

Next, observed lipophilicity and water solubility characteristics of *S. platensis* phytoconstituents (Table 4 and 5)
| Compounds                                                                 | Log S | Solubility Class |
|---------------------------------------------------------------------------|-------|-----------------|
| Ethyl 9-hexadecenoate                                                    | 4.51  | Soluble         |
| Dodecanoic acid, ethyl ester                                             | 3.75  | Moderately      |
| 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-               | 4.71  | Poorly          |
| Methyl gamma.-linolenate                                                 | 4.81  | Poorly          |
| Ethyl linoleate                                                          | 5.03  | Poorly          |
| 9-Octadecenoic acid (Z)-                                                | 4.27  | Poorly          |
| Octadecanoic acid, ethyl ester                                           | 5.47  | Poorly          |
| Hexadecanamide                                                          | 3.87  | Poorly          |
| Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester                       | 7.90  | Poorly          |
| Hexadecenenitrile                                                        | 4.14  | Poorly          |
| Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl est                  | 4.50  | Poorly          |
| 9-Octadecanamide                                                        | 4.22  | Poorly          |
| 7,10-Octadecadienoic acid, methyl ester                                  | 4.57  | Poorly          |
| Octadecanamide                                                          | 4.20  | Poorly          |
| N-Tetradecanoic acid amide                                               | 3.35  | Poorly          |
| Dotriacontane                                                           | -17.14| Insoluble       |
| 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl                | -2.34 | Soluble         |
| Pentadecane                                                             | -7.58 | Poorly          |
| Octadecane                                                              | -9.27 | Poorly          |
| Propionic acid, 3-(2-Methylcyclohexyl)-, ethylester                       | -4.90 | Poorly          |
| Neophytiadiene                                                          | -9.53 | Poorly          |
| 2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-                   | -9.35 | Poorly          |
| 3,7,11,15-Tetramethyl-2-hexadecen-1-ol                                   | -8.47 | Moderately      |
| Hexadecanoic acid, methyl ester                                          | -7.76 | Poorly          |
| Ethyl 9-hexadecenoate                                                   | -7.31 | Poorly          |
| Dodecanoic acid, ethyl ester                                             | -6.03 | Poorly          |
| 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-              | -8.47 | Moderately      |
| Methyl gamma.-linolenate                                                 | -6.46 | Poorly          |

**Table 5.** Water solubility characteristics of the phytoconstituents of *S. platensis* [28]
Then pharmacokinetics parameters, bioavailability and druglikeness according to Lipinski rules also evaluated (Table 6 and 7).

**Table 6. Pharmacokinetics parameters and bioavailability of the phytoconstituents of S. platensis**

| Compounds                                                                 | GI absorption | BBB permeant | Bioavailability Score |
|---------------------------------------------------------------------------|---------------|--------------|-----------------------|
| Ethyl linoleate                                                           | -7.72         | 5.88e-06     | 1.90e-08 Poorly       |
| 9-Octadecenoic acid (Z)-                                                 | -8.26         | 1.54e-06     | 5.46e-09 Poorly       |
| Octadecanoic acid, ethyl ester                                          | -9.40         | 1.24e-07     | 3.97e-10 Poorly       |
| Hexadecanamide                                                           | -7.22         | 1.53e-05     | 6.00e-08 Poorly       |
| Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester                       | -15.65        | 1.27e-13     | 2.24e-16 Insoluble    |
| Hexadecenenitrile                                                        | -7.12         | 1.80e-05     | 7.63e-08 Moderately   |
| Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester               | -7.32         | 1.57e-05     | 4.74e-08 Poorly       |
| 9-Octadecanamide                                                        | -7.71         | 5.49e-06     | 1.95e-08 Poorly       |
| 7,10-Octadecadienoic acid, methyl ester                                  | -7.18         | 1.94e-05     | 6.60e-08 Poorly       |
| Octadecenamide                                                           | -8.18         | 1.87e-06     | 6.66e-09 Poorly       |
| N-Tetradecanoic acid amide                                               | -6.12         | 1.72e-04     | 7.55e-07 Poorly       |

**Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly**

GI absorption - Gastrointestinal absorption; BBB permeant – blood brain barrier permeation
Table 7. Druglikeness rules score of the phytoconstituents of *S. platensis*

| Compounds | A | B | C | D | E | F |
|-----------|---|---|---|---|---|---|
| Dotriacontane | Yes | No | Yes | Yes | Yes | Yes |
| 2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl Pentadecane | Yes | Yes | Yes | Yes | Yes | Yes |
| Octadecane | Yes | No | Yes | Yes | Yes | Yes |
| Propionic acid, 3-(2- Methylenehexyl)-, ethylester | Yes | Yes | Yes | Yes | Yes | Yes |
| Neophytdiene | Yes | No | Yes | Yes | Yes | Yes |
| Ethyl 2-Hexadecene, 3,7,11,15-tetramethyl-[R-[R*,R*- (E)]]-3,7,11,15-Tetramethyl-2-hexadecen-1-ol | Yes | No | Yes | Yes | Yes | Yes |
| Hexadecanoic acid, methyl ester | Yes | No | Yes | Yes | Yes | Yes |
| Ethyl 9-hexadecenoate | Yes | No | Yes | Yes | Yes | Yes |
| Dodecanoic acid, ethyl ester | Yes | Yes | Yes | Yes | Yes | Yes |
| 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-[R-[R*,R*- (E)]]-Methyl gamma.-linolenate | Yes | No | Yes | Yes | Yes | Yes |
| Ethyl linoleate | Yes | No | Yes | Yes | Yes | Yes |
| Ethyl linolate | Yes | No | Yes | Yes | Yes | Yes |
| Octadecanoic acid, ethyl ester | Yes | No | Yes | Yes | Yes | Yes |
| Hexadecanamide | Yes | Yes | Yes | Yes | Yes | Yes |
| Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester | No | No | Yes | Yes | Yes | Yes |
| Hexadecenenitrile | Yes | No | Yes | Yes | Yes | Yes |
| Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester | Yes | Yes | Yes | Yes | Yes | Yes |
| 9-Octadecanamide | Yes | No | Yes | Yes | Yes | Yes |
| 7,10-Octadecadienoic acid, methyl ester | Yes | No | Yes | Yes | Yes | Yes |
| Octadecenamide | Yes | No | Yes | Yes | Yes | Yes |
| N-Tetradecanoic acid amide | Yes | Yes | Yes | Yes | Yes | Yes |

A - molecular mass less than 500 Dalton; B - high lipophilicity (expressed as LogP less than 5); C - less than 5 hydrogen bond donors; D - less than 10 hydrogen bond acceptors; E - molar refractivity should be between 40-130; F - Overall.

3.2. Discussions

Table 1 shows that *S. platensis* extract produced twenty-four compounds with different percentages of compounds from 100% of the total percentage of compounds. *S. platensis* extract contains twelve compounds with a percentage content of >1%, namely, Octadecane (9.02%), Neophytadiene (3.21%), 2-Hexadecene, 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (1%), Ethyl 9-hexadecenoate (2.05%), Dodecanoic acid, ethyl ester (27.71%), 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-[R-[R*,R*- (E)]]- (6.92%), 3,7,11,15-Tetramethyl-2-hexadecen-1-ol (1,44%), Methyl gamma. -linolenate (8.04%), Ethyl linoleate (19.47%), 9-Octadecenoic acid (Z)- (1.47%), Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester (2, 68%), 9-Octadecenamide (1.15%), and Octadecenamide (10.99%). Dodecanoic acid, ethyl ester (27.71%) is a compound with a high percentage of *S. platensis* extract.

Dodecanoic acid, ethyl ester, or ethyl dodecanoate in the extract of *S. platensis* is the compound with the highest relative content of 27.71%. Ethyl dodecanoate compounds in leaf extract (*Coleus blumei*) have the antimicrobial and antioxidant potential [29]. Ethyl dodecanoate compounds have potential as anti-cancer [30], anti-candida [31], mycelial growth inhibition [32]. While the next most
abundant compound is Ethyl linoleate, with a concentration of 19.47%. Ethyl linoleate has potential anti-inflammatory [33], anti-atherosclerotic [34], antibacterial [35], anti-acne agent [36], anti-oxidative activity, and free radical scavenging activity [37], anti-diabetic activity, and lowering serum, total cholesterol [38], anti-melanogenesis [39], anti-atherogenic effect [40]. 9-Octadecenamide and octadecenamide are the most abundant compounds after ethyl dodecanoate and ethyl linoleate. The compound is also called Oleamide. Oleamide compounds have potential as anti-Alzheimer’s Disease [41], anti-depressive [42], Anti-Biofouling [43], Anti-inflammatory Activity [44], anti-metastatic [45]. Anti-epileptic and neuroprotective [46].

Table 3 shows the physicochemical properties of the phytoconstituents of *S. platensis*. Clean molecular and physicochemical properties such as molecular formula, molecular weight, number of heavy atoms, number of aromatic heavy atoms, number of rotatable bonds, number of H-bond acceptors, number of H-bond donors, molar refractivity, and TPSA are all included in this section. Open babel version 2.3.0 was used to calculate the results [47]. The PSA is computed using a fragmental technique known as topological polar surface area (TPSA) and polar atoms sulfur and phosphorus [48]. General characteristics of the phytoconstituents of *S. platensis* revealed all the compounds having molecular weight less than 500 Da, which is a prime property to be called as drug likeness of the small molecules.

Table 4 shows lipophilicity characteristics of the phytoconstituents of *S. platensis*. SwissADME provides five freely available models to evaluate the lipophilicity character of a compound, namely XLOGP3, WLOGP, MLOGP, SILICOS-IT, and iLOGP. [49] XLOGP3, an atomistic approach with corrective factors and a knowledge-based library. WLOGP [50] is a purely atomistic method that is applied to a fragmental system. MLOGP [51, 52], an archetype of the topological method, is based on a linear relationship with 13 molecular descriptors implemented. SILICOS-IT is a hybrid method that relies on 27 fragments and seven topological descriptors. iLOGP is a physics-based method that uses the generalized-born and solvent accessible surface area (GB/SA) model to calculate solvation free energies in n-octanol and water. The arithmetic mean of the values predicted by the five proposed methods [53] is the consensus log P o/w.

Table 5 shows water solubility characteristics of the phytoconstituents of *S. platensis*. Two of the 24 insoluble compounds, namely Dotriacontane and Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester (concentration 0.95%). Most of the compounds were poorly soluble, with 61.56%, and the remaining 36.87% were moderately soluble. SwissADME to predict water solubility, one of which was adopted from Ali [54] (Solubility class: Log S Scale: Insoluble < -10 poorly < -6, moderately, < -4 soluble, < -2 very, < 0 highly). The solubility of a compound is strongly influenced by the solvent used and the ambient temperature and pressure. The saturation concentration is defined as the point at which adding more solute does not increase its concentration in the solution [55,56]. When the highest dose strength is soluble in 250 mL or less of aqueous media over a pH range of 1 to 7.5, it is considered highly soluble. The 250 mL volume estimate is based on standard bioequivalence study protocols, which call for administering a drug product to fasting human volunteers with a glass of water [57]. The decimal logarithm of the molar solubility in water calculates all predicted values (log S). Solubility in mol/l and mg/ml and qualitative solubility classes are also available from SwissADME.

Table 6 shows pharmacokinetics parameters and bioavailability of the phytoconstituents of *S. platensis*. Fifteen compounds (76%) of the *S. platensis* extract had high values for GI absorption. This is directly proportional to the permeant BBB, where 15 compounds (76%) of the *S. platensis* extract. This means that most of the compounds in the *S. platensis* extract have very good absorption. The Egan egg, which was used to assess the predictive power of the model for GI passive absorption and prediction for brain access by passive diffusion to lay the BOILED-Egg finally, is an elliptical region populated by well-absorbed molecules (Brain or Intestinal L Estimate D permeation predictive model). The BOILED-Egg model generates a quick, spontaneous, efficient, yet boisterous method for predicting passive GI absorption, which is helpful for drug discovery and development [58,59].
white region contains molecules that are more likely to be absorbed by the GI tract, while the yellow area (yolk) includes molecules that are more likely to permeate to the brain [60].

Table 7 shows druglikeness rule score of the phytoconstituents of *S. platensis*. All compounds in the extract of *S. platensis* met the druglikeness according to Lipinski's rules. The Lipinski filter (Pfizer) is the first of five rules that characterize small molecules based on physicochemical property profiles such as Molecular Weight (MW) less than 500, MLOGP ≤ 4.15, N or O ≤ 10, NH or OH ≤ 5. All nitrogens and oxygens with at least one hydrogen are considered H-bond acceptors by Lipinski. All nitrogens and oxygens with at least one hydrogen are considered H-bond donors. Furthermore, aliphatic fluorines are acceptors, whereas aliline nitrogen is neither a donor nor an acceptor [61].

4. Conclusions
This study findings that *Sprilulina platensis* extract produced twenty-four compounds. The potential biological activity of the phytoconstituents of *S. platensis* is antimicrobial, antioxidant, anti-cancer, anti-candida, mycelial growth inhibition, anti-inflammatory, anti-atherosclerotic, antibacterial, anti-acne agent, anti-oxidative activity, free radical scavenging activity, anti-diabetic activity, anti-melanogenesis, anti-atherogenic effect, anti-Alzheimer's Disease, anti-depressive, anti-biofouling, anti-metastatic, anti-epileptic and neuroprotective. All compounds in the extract of *S. platensis* met the druglikeness according to Lipinski's rules. The ADME analysis results indicated that *S. platensis* extracts could be developed as traditional medicine and nutraceutical products. It can be the basis of subsequent studies in vitro and in vivo.

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