



Received on 27 April 2025; received in revised form, 13 May 2025; accepted, 14 June 2025; published 01 October 2025

## IN-VITRO AND IN-SILICO STUDY OF BUTEA MONOSPERMA FLOWER

Shikha Rani<sup>1,2</sup>, Vipin Kumar Verma<sup>3</sup>, Neeta Sehgal<sup>4</sup> and Om Prakash<sup>\*4</sup>

Department of Zoology<sup>1</sup>, Kalindi College, University of Delhi, Delhi - 110008, New Delhi, India.

Department of Zoology<sup>2</sup>, University of Delhi, Delhi - 110007, New Delhi, India.

Cardiovascular Pharmacology Lab<sup>3</sup>, Department of Pharmacology, All India Institute of Medical Sciences, Delhi - 110029, New Delhi, India.

Department of Zoology<sup>4</sup>, Sri Venkateswara College, University of Delhi, Delhi - 110021, New Delhi, India.

### Keywords:

*Butea monosperma*, Antioxidants, Phytochemicals, Secondary metabolite, GC-MS, Phenol, Flavonoid, Antidiabetic, Autodock tool

### Correspondence to Author: Prof. Om Prakash

Professor,  
Department of Zoology,  
Sri Venkateswara College,  
University of Delhi, Delhi - 110021,  
New Delhi, India.

**E-mail:** opchanna@gmail.com

**ABSTRACT:** The active compounds present in plants gained attention for their biological activity and this makes them important for the pharmaceutical industries. *Butea monosperma* has significant role in traditional medicines. Its leaves, bark, and flower have an important role against diabetes, filariasis, ulcers, inflammations, etc. However, till date no detailed phytochemicals profiling in flowers of *B. monosperma* along with their antioxidant and antidiabetic potential has reported. This study aims to measure antioxidant activity, total phenols, flavonoid contents in methanol and ethanol extract of the flower, and to identify their compounds through Gas Chromatography-Mass Spectrometry (GC-MS) analysis. Biological activity was determined by available literature present on NCBI, PubChem. However, Antioxidant actions were measured by DPPH and FRAP assays. Further antidiabetic potential of compound extract was analyzed using *in-silico* approach. It was found that methanolic extract showed better antioxidant potential than ethanolic extract. Total Phenol and flavonoid content were investigated but no significant difference was observed between the extracts. 42 major compounds were identified in methanolic extract using GC-MS, among which, 30 have well-reported structures and biological activities. D-Pinitol, present in methanolic extract at higher concentration were used for docking analysis to confirm their anti-diabetic properties by inhibiting the alpha amylase activity. This is the first report on antidiabetic potential of methanol extract of *B. monosperma* using *in-silico* approach. The results provide valuable data on the phytochemicals and their biological potential that can be further used for the treatment of other diseases where oxidation and inflammation play a significant role.

**INTRODUCTION:** A few phytochemical compounds, also referred to as secondary metabolites, are present in different kinds of plants, have pivotal contribution in the pharmaceutical industries.

There is a diverse array of phytochemical compounds such as flavonoids, tannins, phenols, and terpenoids<sup>1, 2</sup>. These compounds have multifaceted medical effects including antibacterial, anti-inflammatory, and anti-apoptotic properties etc<sup>3</sup>.

WHO has notably highlighted the significant reliance of 70% of Asian and African countries dependence on herbal medicines prepared from plant sources<sup>4</sup>. These medicines are recommended because of their affirmative effects, low costs, easy availability, and fewer side effects<sup>5, 6</sup>.

<p><b>QUICK RESPONSE CODE</b></p>  <p>DOI link: <a href="https://doi.org/10.13040/IJPSR.0975-8232.16(10).2783-93">https://doi.org/10.13040/IJPSR.0975-8232.16(10).2783-93</a></p>	<p><b>DOI:</b> 10.13040/IJPSR.0975-8232.16(10).2783-93</p> <p>This article can be accessed online on <a href="http://www.ijpsr.com">www.ijpsr.com</a></p>
--	---

The use of these active compounds as a medicine is not limited to only humans but it has been used for various other animals<sup>7, 8</sup>. These active compounds are immunomodulatory as they promote both humoral and cell-mediated responses in an organism<sup>9, 10</sup>. Not only plants, but algae, lichens, and yeast also promote the use of herbal medicines in Ayurveda, Unani, and other local health practices<sup>11</sup>. Compounds have antioxidant properties because of which they serve as protective agents by counteracting oxidative stress through the reduction of free radicals, thereby mitigating the progression of cellular damage<sup>12, 13</sup>.

For many years, research has emphasized more on elucidating the identification and biological function of active compounds found present in plant parts. The focus of this study is to identify and explore the phytochemical properties of *Butea monosperma* flower. *B. monosperma* (Family: Fabaceae) is a flower-bearing tree also called palash (in India) or flame of the forest because of the appearance of the flower<sup>14, 15</sup>.

This species belongs to one of the largest families of flowers, encompassing approximately 1800 species. It is indigenous to South Asian regions like India, Nepal, Bangladesh, Myanmar, Thailand, Sri Lanka, Pakistan, and Indonesia. It is a deciduous tree which typically blooms during late winter. It has been used in Ayurvedic, Unani, and Homeopathic medicines because of various beneficial effect on night blindness, ulcers, filariasis, and many more<sup>16</sup>. It is employed in the treatment of various other disease conditions like antifertility, cancer, convulsions, diabetes, and oxidative stress<sup>15, 17, 18</sup>.

Diabetes mellitus is a concern for public health sector as it is the third most common chronic disease worldwide, surpassed by cancer and cardiovascular diseases<sup>19, 20</sup>. Dysregulation in the metabolism of carbohydrates, fats, and proteins, primarily arising from insufficient insulin production or resistance to insulin action caused this metabolic disorder. This results in hyperglycaemia which can lead to range of severe complications in multiple organs like liver, pancreases, intestine, and stomach<sup>21, 22</sup>. Alpha amylase is an enzyme secreted by the pancreas, responsible for hydrolyses of starch into small

sugars, these small sugars converted into glucose and absorbed into bloodstream subsequently<sup>23, 24</sup>. This contributes to elevated postprandial blood glucose levels. Dysregulation or hyperactivation of alpha amylase can exacerbate glucose levels and thereby increasing the potential of insulin resistance and development of type 2 diabetes. So, inhibiting the potentials of alpha amylase is an effective way for reducing the risk of hyperglycemia<sup>25</sup>.

There are various oral agents available for the management of diabetes but achieving therapeutic efficiency without adverse effect remains a challenge for the medical sector. Metformin is a well-established first line pharmacological agent for diabetes management<sup>26-28</sup> basically known for inhibiting alpha-amylase activity by reducing hepatic gluconeogenesis and improving peripheral insulin sensitivity. However, there are certain side effects that affects various organs, particularly in the liver, intestine, and gastrointestinal organs. Adverse effects include discomfort in abdomen, nausea, and lactic acidosis<sup>29, 30</sup>.

Taking the context of earlier studies, flowers of *B. monosperma* were used for the investigation of antioxidant potentials and their antidiabetic properties. The present work aims to evaluate the efficiency of methanol and ethanol extract from the flower of *B. monosperma*. Our objectives include the evaluation of phenol and flavonoid concentration, elucidate the antioxidant potential through DPPH and FRAP assay.

Furthermore, the phytocomponents were identified by using GC-MS and pursued to characterize the biological activities of the active compounds found in extracts of *B. monosperma* flower. Also, study of the alpha amylase inhibiting properties of compounds presents in flowers of *B. monosperma* by performing docking with alpha amylase enzyme using Autodock tool.

## EXPERIMENTAL:

**Collection of Flowers:** Flowers of *Butea monosperma* (Accession number DUH15968) were collected from the district of Mirzapur, Uttar Pradesh (24.8675° N, 82.8556° E) between February to April. Selected flowers were thoroughly washed with tap water and dried at

room temperature. Samples were ground into fine powder, passed through a sieve for uniform powder, and stored at -20°C.

**Preparation of Extracts:** 10g of powder was weighed and dissolved in 100ml of methanol and ethanol solvents separately by maceration process for 24 hours on magnetic stirrer. Both the slurry obtained were filtered using Whatman filter paper No. 1. The collected solvents (filtrates) were further dried using rotary evaporator at 40°C, and the extracts were weighed, and stored at -20°C until further use. The concentrated stocks (10mg/ml) were used further for antioxidant assays and phytochemical screening.

#### Antioxidant Assays:

**DPPH (2,2-Diphenyl-1-Picrylhydrazyl) Assay:** DPPH assay is a radical scavenging assay performed using the standard protocol<sup>31, 32</sup>. *B. monosperma* flower extract was dissolved in both methanol and ethanol at a final concentration of 1mg/ml.

DPPH solution ( $6 \times 10^{-5}$  M) was prepared in methanol solvent and added to both the samples equally, followed by incubation in dark condition for 30 minutes. Ascorbic acid was taken as positive control and the blank contains the same amount of DPPH solution and distilled water. Absorbance was recorded at 515nm. All the reactions were performed in triplicates. The free radical scavenging property was recorded according to the formula

$$\% \text{ Inhibition} = (A_2 - A_1) / A_2 \times 100$$

Where, A1 is the absorbance of extract solution after 30 minutes and A2 is the absorbance of blank solution.

**FRAP (Ferric Reducing Antioxidant Power) Assay:** For FRAP assay, 5µl of plant extract (1mg/ml) of both the solvents were mixed with 200µl of FRAP reagent containing 300mM acetate buffer, 10mM 2,4,6-tripyridyl triazine in 40mM HCl, and 20mM ferric chloride in ratio of 10:1:1 respectively, adjusted to pH 3.6. Samples were then incubated for 20 minutes at 37°C. Ferrous sulphate was used for the standard curve. Absorbance was recorded at 593nm taking acetate buffer as control<sup>33, 34</sup>.

**Total Phenol Content (TPC):** 1ml of extract (10mg/ml) was dissolved in 500µl of Folin-Ciocalteu reagent and mixed well. 1.5ml of sodium carbonate solution (20%) was mixed after 1 minute followed by incubation for 2 hours at room temperature in the dark. The flower samples were exchanged with equal amounts of methanol and ethanol in the blank. Gallic acid was taken as standard and absorbance was measured for all solutions at wavelength of 750nm by using UV-Spectrophotometer<sup>33, 34, 35</sup>.

**Total Flavonoid Content (TFC):** TFC was estimated by using the protocol mentioned in reference<sup>33</sup>, 1ml of extract (10mg/ml) was mixed with 1ml of 2% Aluminium chloride. Absorbance was recorded after 20 minutes of incubation at room temperature at 415nm. A standard curve was plotted using quercetin and a blank sample using distilled water. The flavonoid content was expressed in µg QEs/mg (QE= quercetin equivalents).

**Gas Chromatography-Mass Spectrometry (GC-MS):** The methanol extract of *B. monosperma* flower were analyzed using a thermal desorption TD-20 system, GCMSQP-2010 Plus (Shimadzu, Japan) fitted with RTX-5MS column (30m × 0.25mm inner diameter × 0.25µm film thickness) operated at 70eV electron impact mode. Helium was used as a carrier gas at 99.99% purity. Column Temperature was started at 80°C and reached 300°C with a gradual increase of 5°C per minute and pressure was maintained at 80kpa. The Mass spectrum was attached to the system with a scan range of 40 m/z to 650 m/z scan interval of 0.50 seconds.

**GC-MS Data Interpretation:** The phytochemicals were identified based on their area percentage of mass spectra, retention time, and percentage of peak area and its comparison with the data of library of NIST11.LIB of National Institute of Standards and Technology (NIST) MS programme v.2.0d and WILEY08 libraries were used along with their names, chemical formulas, molecular weight, structure of components. Unknown components were also identified by using Wiley libraries based on their spectrum. The biological and chemical activities were identified by using NCBI-Pubchem and various literatures.

**Autodocking Analysis:** The molecular docking was performed for the highly available compound i.e. D-Pinitol, in methanol extract of *Butea monosperma*. The 3D structure of  $\alpha$ -amylase were obtained from the Research Collaboratory for Structural Bioinformatics (RCSB) ProteinData Bank (PDB) at (<https://www.rcsb.org/>) with PDB IDs 1B2Y. Protein structure were prepared Using Autodocktools 1.5.7 software doing various modifications like removal of water, assigning hydrogen bonds, distribution of charges and flexible torsions followed by setting grid nearby the docking site.

**Ligand Structural Retrieval:** The chemical structures of D-Pinitol compound is retrieved from NCBI PubChem compound database (<https://pubchem.ncbi.nlm.nih.gov/>) and saved in sdf format. It was further converted into .pdb file using Open Babel software.

**Docking and Analysing:** The prepared protein and ligand were docked using AutoDock tool 1.5.7. Ten different conformations of different binding energies were generated from Protein-Ligand interaction. The one with the lowest binding energy was more stable and selected for the virtual screening using Discovery Studio 2021 tool. 2D structures were generated to check name of atomic acids and their position to which ligands bind and to check the different kind of bonds between protein binding site and ligands.

**Statistical Analysis:** Statistical differences were calculated by Student T-test using SigmaPlot 12.0 software where  $p\text{-value} \geq$  were considered significant. The requisite sample size was maintained throughout the study.

**RESULTS AND DISCUSSION:** In recent years plants with more antioxidant potential have gained a lot of attention. These antioxidant compounds reduce the adverse events because of oxidative stress. Oxidative stress occurs due to insufficient availability of antioxidants and this affects the defense system of the body that can lead to the occurrence of various diseases<sup>36</sup>.

**Phytochemical Extraction and Analysis:** Plant extracts contain a variety of phytochemical compounds such as phenols, flavonoids, tannis, phytol and essential oils etc. Efficiency of these

compound extraction depends on the type of solvent used. Here Methanol and ethanol solvent were used for the extraction of phytochemical from the flower of *B. monosperma*.

The extracted content was 5.67g and 3.91g in methanol and ethanol respectively. So, the content was extracted more in methanol as compared to ethanol. As methanol being a polar solvent and higher dielectric constant with a smaller molecular size demonstrates an efficient extraction for phytochemicals. A similar qualitative observation was seen in some studies<sup>37</sup>.

Various other tests have also been performed to highlight the presence of phenols, flavonoids, tannins, and various other metabolites in these extracts. On the other side, ethanol has lower polarity due to its longer hydrocarbon chain that makes ethanol less effective for extracting highly polar compounds compared to methanol.

**Antioxidant Assay:** Antioxidants activity of extracted compound is measured to know the potentials of phytochemicals to neutralize the free radicals and mitigating the oxidative stress. Radical scavenging assay of methanol and ethanol extract of *B. monosperma* flower was performed using DPPH and FRAP assay using ascorbic acid and ferrous sulphate as positive standards respectively. DPPH assay is the most common method to determine the antioxidant ability of the compounds, free radicals are eliminated by the antioxidants present in the extract of flower and leads to discoloration of DPPH compound<sup>38</sup>.

This assay is simple, rapid, and sensitive, makes it one of the useful techniques to estimate the antioxidant potentials. The electron of nitrogen atom present in DPPH is reduced into hydrazine by taking the hydrogen from the antioxidants present in compounds<sup>39</sup>.

Similar reactions occurred in both the extracts although the intensities were different. Antioxidant activity exhibited by methanol extract was significantly higher than ethanol extract of *B. monosperma* as well as standard ascorbic acid **Table 1**. Similar results were observed in *Mentha piperrascens* and *Moringa stenopetala*, where methanol extract has more antioxidant potential than ethanol and water extracts<sup>40, 41</sup>.



**TABLE 1: DPPH AND FRAP ASSAY IN METHANOL AND ETHANOL EXTRACTS OF *B. MONOSPERMA* FLOWER**

	DPPH Assay (% scavenging activity)	FRAP Assay (ug gallic acid/mg extract)
	Mean $\pm$ SEM	Mean $\pm$ SEM
Methanol extract	61.529 $\pm$ 2.532 <sup>a</sup>	3.454965 $\pm$ 0.442 <sup>a</sup>
Ethanol extract	34.06 $\pm$ 4.365 <sup>b</sup>	1.2840 $\pm$ 0.222 <sup>b</sup>
Ascorbic acid	57.496 $\pm$ 2.555	-
Gallic acid	-	2.076 $\pm$ 0.081

Values are expressed in Mean  $\pm$  SEM and Superscripts <sup>a</sup> and <sup>b</sup> represents the significant difference between both the extracts.

In FRAP Assay, the higher concentration of antioxidants reduces more ferric ions into ferrous ions and forms blue coloured solution. The intensity of colour is directly proportional to the reducing power of compound. Although both the extracts showed positive results for FRAP assay **Table 1**, there is a significant difference between both the extracts i.e. methanol showed higher reducing potential than ethanol extract. These results showed that methanol extract has significantly more antioxidant potential than ethanol extract. However, in some plants like ethanolic extract of *R. coreanu* and water extract of *M. piperascens* has higher FRAP value than methanolic extract. So, the FRAP value is not always constant for the solvent. It changes with respect to their components showing antioxidant potential <sup>41, 42</sup>.

**Total Phenolic Content:** Secondary metabolites are majorly phenolic compounds, present in plants.

They are aromatic compounds to which one or more hydroxyl group has attached <sup>43, 44</sup>. It has various biological functions to play that help plants physiologically and morphologically like growth, repair, protection against pathogens, etc <sup>45</sup>. Phenols reduce the Folin-Ciocalteu reagent in the extracts and produce blue color molybdenum-tungsten that is measured spectrophotometrically at 760nm. Its intensity increased with the increase in phenolic content. No significant differences were found in the level of phenols in both the extracts of *B. monosperma* flower **Table 2**.

**Total Flavonoid Content:** Flavonoids were measured by taking quercetin as a standard. Both the extracts showed the presence of flavonoids but there was no significant difference in the level of flavonoid. Concentration of flavonoid was expressed in microgram equivalent quercetin per mg extract **Table 2**.

**TABLE 2: TOTAL PHENOLIC CONTENT AND TOTAL FLAVONOID CONTENT IN METHANOL AND ETHANOL EXTRACTS OF *B. MONOSPERMA* FLOWER**

	Total Phenolic (μg gallic acid/mg extract)	Total Flavonoid (μg quercetin/mg extract)
	Mean $\pm$ SEM	Mean $\pm$ SEM
Methanol extract	17.31 $\pm$ 0.91 <sup>a</sup>	4.15 $\pm$ 0.283 <sup>b</sup>
Ethanol extract	17.05 $\pm$ 2.43 <sup>a</sup>	3.26 $\pm$ 0.332 <sup>b</sup>

Values are expressed in μg equivalents to gallic acid and quercetin respectively. Values are expressed in Mean  $\pm$  SEM and Superscripts <sup>a</sup> and <sup>b</sup> represents the significant difference between both the extracts.

**GC-MS Data Interpretation:** During data interpretation of gas chromatography Retention time, peak size and area percentage were taken as a base for the identification of the compounds represented by different peaks. Peaks were compared with the data of NIST11.LIB of National Institute of Standards and Technology (NIST) MS program v.2.0d and WILEY08 libraries for their identification. More number of peaks and their respective compounds in methanol extract have well-established anti-oxidant, anti-inflammatory, and immune-modulatory properties which are in-line with our biochemical estimation of antioxidant potential, therefore, detailed structures, chemical

formula, and biological activities of the compounds were identified only of methanol extract using the NCBI-PubChem. Methanolic extract of *B. monosperma* flower resolved in 42 peaks as shown in the chromatogram **Fig. 1**, representing various phyto-compounds and secondary metabolites. The chromatogram also gives an approximate percentage of compounds present in extracts. Out of 42 compounds, only 30 were identified based on their relative abundance, for their chemical structure, chemical formulae, and biological activity as shown in **Table 3** with the help of NCBI PubChem.

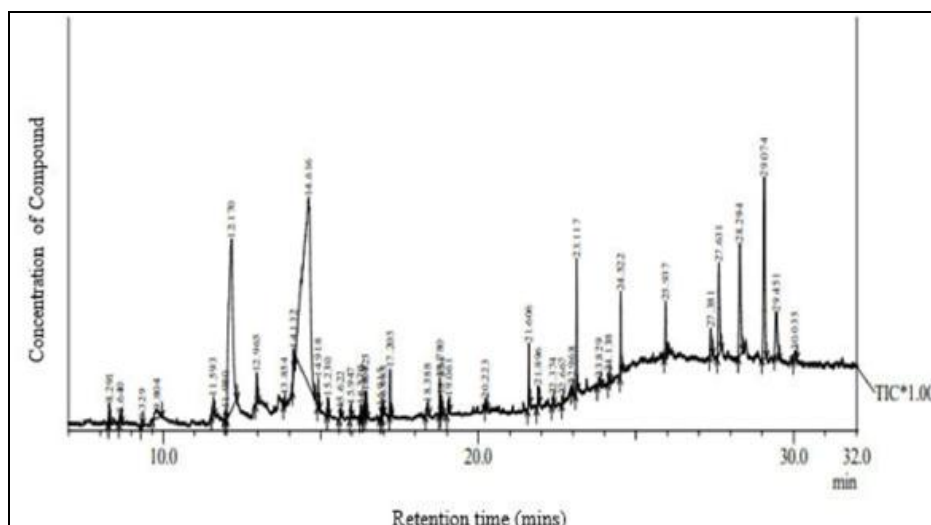


FIG. 1: GC CHROMATOGRAM OF METHANOL EXTRACT OF *B. MONOSPERMA* FLOWER DERIVED FROM GC-MS

TABLE 3: LIST OF PHYTO-COMPOUNDS DERIVED FROM GC-MS OF METHANOL EXTRACT OF *B. MONOSPERMA* FLOWER

Peak	Retention time (min)	Area %	Common name	Chemical Formula	Biological activity
1	8.291	0.39	1,2-di-tert-Butylbenzene	C <sub>14</sub> H <sub>22</sub>	-
3	9.329	0.07	Docosane	C <sub>22</sub> H <sub>46</sub>	-
4	9.804	1.00	1,3-Benzenediol	C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>	Apoptotic, Anti-angiogenetic <sup>46</sup>
5	11.593	0.58	Sulfurousacid,2-ethylhexylhexylester	C <sub>14</sub> H <sub>30</sub> O <sub>3</sub> S	Acidifier <sup>47</sup>
7	12.170	20.27	D-Allose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	Anticancer, Immunomodulatory <sup>48</sup> ,Antitumour <sup>49</sup>
8	12.965	1.05	1,2-BenzenedicarboxylicAcid,DiethylEster	C <sub>8</sub> H <sub>6</sub> O <sub>4</sub>	Antibacterial <sup>50</sup>
10	14.132	0.62	Eicosane	C <sub>20</sub> H <sub>42</sub>	Antiinflammatory, Analgesic, Antipyretic <sup>51</sup>
11	14.616	40.86	Mome Inositol	C <sub>7</sub> H <sub>14</sub> O <sub>6</sub>	Antialopethic <sup>40</sup> , Anticirrhotic <sup>40</sup> , Antineuropathic, Cholestrolytic <sup>52,53</sup> , lipotrophic
12	14.918	0.67	Tetra-decanoicacid	C <sub>14</sub> H <sub>28</sub> O	Antioxidant, Antidiabetic, Antiviral <sup>54</sup>
14	15.622	0.19	Neophytadiene	C <sub>20</sub> H <sub>38</sub>	Anti-inflammatory <sup>55</sup>
15	15.947	0.24	1,2-BenzenedicarboxylicAcid,DibutylEster	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	Antibacterial <sup>56</sup>
17	16.369	0.24	Hexadecane	C <sub>16</sub> H <sub>34</sub>	Antitumour <sup>57</sup> , Antibacterial <sup>57</sup> Anti-inflammatory <sup>58</sup>
18	16.425	0.94	(6E,10E)-7,11,15-Trimethyl-3-Methylene-1,6,10,14	C <sub>20</sub> H <sub>32</sub>	-
19	16.915	0.13	PhthalicAcid, butyl tridec-2-yn-1-yl ester	C <sub>25</sub> H <sub>36</sub> O <sub>4</sub>	Insecticidal <sup>59</sup>
20	16.985	0.21	n-Hexadecanoicacid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>	Antioxidant, Antibacterial <sup>60</sup> Anti-inflammatory <sup>61</sup>
23	18.780	0.63	E,E,Z-1,3,12-Nonadecatriene-5,14-diol	C <sub>19</sub> H <sub>34</sub> O <sub>2</sub>	SARS CoV-2 inhibitor <sup>62</sup>
24	18.834	0.36	EthylOleate	C <sub>20</sub> H <sub>38</sub> O <sub>2</sub>	Antioxidant <sup>63,64</sup> , Antiinflammatory <sup>64</sup>
25	19.061	0.46	8-Methylnonanoicacid	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	Antimicrobial <sup>65</sup> , Antibacterial <sup>66</sup>
26	20.223	0.28	Carbonicacid,decylnonylester	C <sub>20</sub> H <sub>40</sub> O <sub>3</sub>	Antimicrobial <sup>67</sup> , Antibacterial <sup>67</sup>
29	22.374	0.15	Eicosane	C <sub>20</sub> H <sub>41</sub> I	Antifungal <sup>68</sup>
31	22.968	0.13	Cyclohexanol,4-(tri-methylsilyl) oxy-, cis-	C <sub>9</sub> H <sub>20</sub> O <sub>2</sub> Si	Antimicrobial <sup>69</sup> , Antifungal <sup>69</sup>
32	23.117	2.61	Hexatriacontane	C <sub>36</sub> H <sub>74</sub>	Anticancer <sup>58</sup> , Antibacterial <sup>72</sup> , Antioxidant <sup>73</sup>
33	23.829	0.27	Sulfurousacid,octadecyl2-propylester	C <sub>21</sub> H <sub>44</sub> O <sub>3</sub> S	Antimicrobial <sup>74</sup> , Antimycobacterial <sup>74</sup>
34	24.138	0.16	Eicosanal	C <sub>20</sub> H <sub>40</sub> O	Anti-depressant <sup>75</sup> , Anxiolytic <sup>75</sup>
37	27.381	0.96	Campesterol	C <sub>28</sub> H <sub>48</sub> O	Antiangiogenic <sup>76</sup> , Antiinflammatory <sup>76</sup>

38	27.631	3.71	Stigmasterol	C <sub>29</sub> H <sub>48</sub> O	Antioxidant <sup>77</sup> , Anti breast cancer <sup>78</sup>
39	28.294	5.07	Sitosterol	C <sub>29</sub> H <sub>50</sub> O	Cancer therapy agent <sup>79</sup> , Antioxidant, hepatoprotective <sup>80</sup>
40	29.074	7.32	Lup-20(29)-en-3-one	C <sub>30</sub> H <sub>48</sub> O	Antileukemic, Antiproliferative
41	29.451	2.41	Lupeol	C <sub>30</sub> H <sub>50</sub> O	Anti-inflammatory, anticancer <sup>81</sup> , cardioprotective agent <sup>82</sup> .
42	30.035	0.30	Pollinastanol	C <sub>28</sub> H <sub>48</sub> O	-

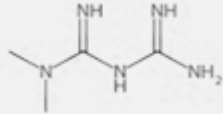
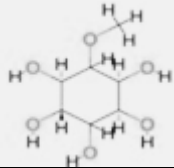
**Docking Analysis:** Managing blood glucose level is an important criterion to manage diabetes. The present work revealed the binding interaction of D-pinitol compound with  $\alpha$ -amylase enzymes or protein molecules.

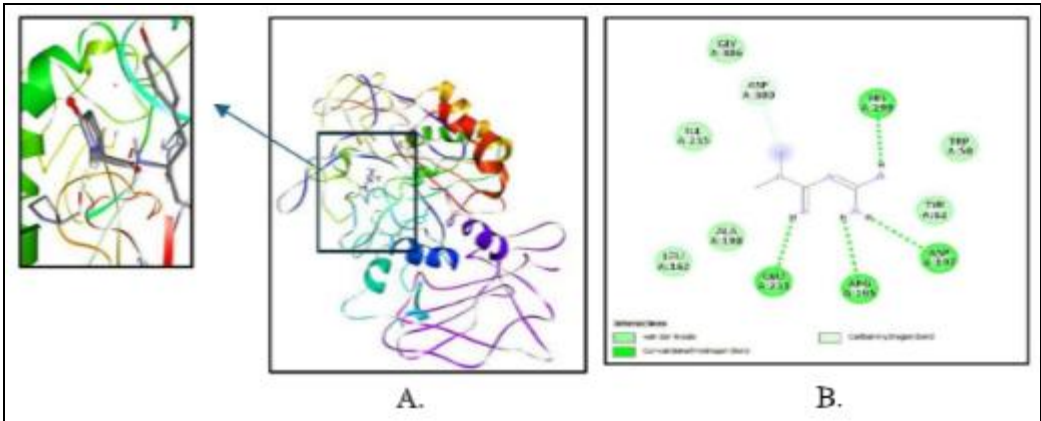
Further, an analysis into the interaction was performed *in-silico* using the Auto Dock Vina tool. Based on GC-MS result, D-pinitol was identified highly available compound in methanol extract of *B. monosperma* and used as a ligand for docking along with metformin (positive control). As revealed in **Table 4**, D-Pinitol showed high binding affinity for alpha amylase enzyme as compared to Metformin. The binding energy of D-Pinitol and metformin is -5.8 kcal/mol and -5.2 kcal/mol

respectively. It is essential to note that the more negative binding free energy value indicates a higher affinity for ligand binding to the receptor as observed in these compound interactions.

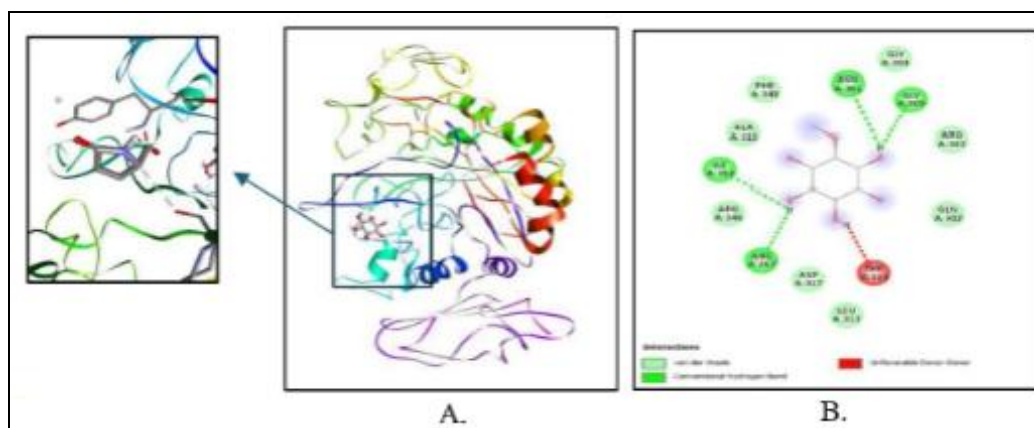
So, it indicates that D-pinitol proved to be better antagonist then metformin against alpha amylase enzyme. The detailed interaction between receptor and ligands interactions were analyzed using free version of Biovia Discovery studio Visualizer 2021 software. This software generates best docking structure, caron interaction, amino acid residues interaction along with bond type. The amino acid residues for alpha amylase with metformin and D-pinitol has been mentioned in table 4 along with 2D structure.

**TABLE 4: STRUCTURE AND PREDICTED BINDING AFFINITY AND DETAILED DOCKING INTERACTIONS OF A-AMYLASE WITH METFORMIN (POSITIVE CONTROL) AND METHANOL EXTRACTED COMPOUND D-PINITOL**

S. no.	Compound name	Chemical Structure	Binding affinity (kcal/mol) with H bond residues
1	Metformin		-5.2 (HIS A:299, ASP A:197, ARG A:195, GLU A:233)
2	D-Pinitol		-5.8 (ALA A:310, ASP A:317, ARG A:267, GLN A:302, THR A:314)



**FIG. 2: METFORMIN COMPOUND DOCKED WITH ALPHA AMYLASE ENZYME (A.) LIGAND INTERACTION HAS SHOWN IN ZOOMED IMAGE. STRUCTURES ARE ALSO PRESENTED IN 2D SHOWING HYDROGEN BONDS (B).**



**FIG. 3: D-PINTOL COMPOUND DOCKED WITH ALPHA AMYLASE ENZYME (A.), LIGAND INTERACTION HAS SHOWN IN ZOOMED IMAGE. STRUCTURES ARE ALSO PRESENTED IN 2D SHOWING HYDROGEN BONDS (B)**

**CONCLUSIONS:** After summarizing the whole study about the antioxidant potential of methanol and ethanol extracts of *B. monosperma* flower, we conclude that methanol extract of *B. monosperma* flower exhibits higher potential biological or medicinal importance as compared to ethanol solvent. Compounds showed presence of phenols and flavonoids that raised the antioxidant potentials of extracts. Presence of momeionistol at higher percentage make this flower a potent candidate for the treatment of type 2 diabetes. The detailed examination of these compounds has unveiled a promising route for further research into their biological activities. Overall, this is the first report on *in-silico* analysis of antidiabetic potential of methanol extract of *Butea monosperma*. These results underscore the advantages of exploring the plant-derived antioxidant as potential remedies against oxidative stress ailments. It might also be helpful in pharmaceuticals, nutraceuticals, and cosmetic industries.

**ACKNOWLEDGMENT:** Shikha Rani is expressing her sincere thanks to the Head of the Department of Zoology, University of Delhi, Principal of Kalindi College, and Sri Venkateswara College, University of Delhi for their continuous support and encouragement to complete the article. Also acknowledge to CSIR institute for the research fellowship.

**CONFLICT OF INTEREST:** No conflict of interest to declare.

## REFERENCES:

1. Awuchi CG: The biochemistry, toxicology, and Uses of the ecologically active phytochemicals: Alkaloids,

terpenes, polyphenols, and glycosides. Merit Research Journals 2020; 5(1): 6-21.

2. Sousa F, Ferreira D, Reis S and Costa P: Current insights on antifungal therapy: Novel nanotechnology approaches for drug delivery systems and new drugs from natural sources. Pharmaceuticals 2020; 13(9): 248. <https://doi.org/10.3390/ph13090248>.
3. Tasneem S, Liu B, Li B, Choudhary MI and Wang W: Molecular pharmacology of inflammation: Medicinal plants as anti-inflammatory agents. Pharmacological Research 2019; 139: 126-40. <https://doi.org/10.1016/j.phrs.2018.11.001>.
4. Verma V, Sehgal N, Kumar Verma V and Prakash O: Characterization, and screening of bioactive compounds in the extract prepared from aerial roots of *Ficus benghalensis*. International Journal of Pharmaceutical Sciences and Research 2015; 6: 1000. [https://doi.org/10.13040/IJPSR.0975-8232.6\(12\).5056-69](https://doi.org/10.13040/IJPSR.0975-8232.6(12).5056-69).
5. Alkahtani J, Elshikh MS, Dwiningsih Y, Rath MA, Sathya R and Vijayaraghavan P: *In-vitro* antidepressant property of methanol extract of *Bacopa monnieri*. Journal of King Saud University Science 2022; 34(8): 102299. <https://doi.org/10.1016/j.jksus.2022.102299>.
6. Dharmraj Ghutke T, ParvinK, Banu R, Bansal S, Srivastava A, Rout S and Ramzan U: A Comprehensive Review on the Therapeutic Properties of Medicinal Plants. Acta Traditonal Medicine 2023; 01: 13. <https://doi.org/10.5281/zenodo.8227509>.
7. Salunkhe AJ and Patil RN: Hepatoprotective effect of ethanolic extract of *Andrographis paniculata* against thioacetamide induced toxicity in the liver of albino rats. Research Journal of Life Sciences, Bioinformatics, Pharmaceutical and Chemical Sciences 2018; 4: 549-59. <https://doi.org/10.26479/2018.0406.43>.
8. El-Saadony MT, Zabermaawi NM, Zabermaawi NM, Burollus MA, Shafi ME, Alagawany M and Abd El-Hack ME: Nutritional aspects and health benefits of bioactive plant compounds against infectious diseases: a review. Food Review International 2023; 39(4): 2138-2160. <https://doi.org/10.1080/87559129.2021.1944183>.
9. Van Doan H, Hoseinifar SH, Harikrishnan R, Khamlor T, Punyatong M, Tapingkae W and El-Haroun E: Impacts of pineapple peel powder on growth performance, innate immunity, disease resistance, and relative immune gene expression of Nile tilapia, *Oreochromis niloticus*. Fish Shellfish Immunology 2021; 114: 311-319. <https://doi.org/10.1016/j.fsi.2021.04.002>.



10. Karami E, Goodarzi Z, Chahardoli R, Ghazi Khansari M, Kiani M and Shahataheri SJ: Investigating the protective effects of aqueous extract of the wormwood plant (*Artemisia absinthium*) on alumina nanoparticle-induced pulmonary toxicity in male Wistar rats. *Journal of Health and Safety at Work* 2022; 12(2): 288-308. <https://creativecommons.org/licenses/by/4.0/>.
11. Ślusarczyk J, Adamska E and Czerwik-Marcinkowska J: Fungi and algae as sources of medicinal and other biologically active compounds: A review. *Nutrients* 2021; 13(9): 3178. <https://doi.org/10.3390/nu13093178>.
12. Stagos D: Antioxidant activity of polyphenolic plant extracts. *Antioxidants* 2020; 9(1): 19. <https://doi.org/10.3390/antiox9010019>.
13. Zuo J, Zhang Z, Luo M, Zhou L, Nice E C, Zhang W and Huang C: Redox signaling at the crossroads of human health and disease. *MedComm* 2022; 3(2): e127. <https://doi.org/10.1002/mco2.127>.
14. Tanaka N and Kashiwada Y: Phytochemical studies on traditional herbal medicines based on the ethnopharmacological information obtained by field studies. *Journal of natural medicines* 2021; 75: 762-783. <https://doi.org/10.1007/s11418-021-01545-7>.
15. Chauhan SS and Mahish PK: Flavonoids of the flame of forest-*Butea monosperma*. *Research Journal of Pharmacy and Technology* 2020; 13: 5647-5653. <https://doi.org/10.5958/0974-360X.2020.00984.1>.
16. Farooq MU, Mumtaz MW, Mukhtar H, Rashid U and Akhtar MT: UHPLC-QTOF-MS/MS based phytochemical characterization and anti-hyperglycemic prospective of hydro-ethanolic leaf extract of *Butea monosperma*. *Scientific Reports* 2020; 10: <https://doi.org/10.1038/s41598-020-60076-5>.
17. Sharma N and Garg V: Antidiabetic and Antioxidant Potential of Ethanolic Extract of *Butea Monosperma* Leaves in Alloxan-Induced Diabetic Mice. *Indian Journal of Biochemistry and Biophysics* 2009; 46. <http://nopr.niscares.in/handle/123456789/3324>
18. Thida M, Moe TS, Chan KN, Ei SL and Khair AA: In vitro antidiabetic activities of Myanmar medicinal plants: *Cassia siamea* Lam. and *Butea monosperma* Roxb. *Indian Journal of Natural Products and Resources* 2022; 13: 483-490 <https://doi.org/10.56042/ijnpr.v13i4.63881>.
19. Deshmukh C D, Jain A and Nahata B: Diabetes mellitus: a review. *International Journal of Pure Applied Biosciences* 2015; 3(3): 224-230.
20. Tomic D, Shaw JE and Magliano DJ: The burden and risks of emerging complications of diabetes mellitus. *Nature Review Endocrinology* 2022; 18(9): 525-539. <https://doi.org/10.1038/s41574-022-00690-7>.
21. Zhao X, An X, Yang C, Sun W, Ji H and Lian F: The crucial role and mechanism of insulin resistance in metabolic disease. *Frontier Endocrinology* 2023; 14: 1149239. <https://doi.org/10.3389/fendo.2023.1149239>.
22. Li M, Chi X, Wang Y, Setrerrahmane S, Xie W and Xu H: Trends in insulin resistance: insights into mechanisms and therapeutic strategy. *Signal Transduction and Targeted Therapy* 2022; 7(1): 216. <https://doi.org/10.1038/s41392-022-01073-0>.
23. Agarwal P and Gupta R: Alpha-amylase inhibition can treat diabetes mellitus. *Research Reviews: Journal of Medical and Health and Sciences* 2016; 5(4): 1-8. <https://www.researchgate.net/publication/321144770>.
24. Kaur N, Kumar V, Nayak S K, Wadhwa P, Kaur P and Sahu SK: Alpha-amylase as molecular target for treatment of diabetes mellitus: A comprehensive review. *Chemical Biology and Drug Design* 2021; 98(4): 539-560. <https://doi.org/10.1111/cbdd.13909>.
25. Agarwal P and Gupta R: Alpha-amylase inhibition can treat diabetes mellitus. *Research and Reviews Journal of Medical and Health Sciences* 2016; 5(4): 1-8. <https://www.researchgate.net/publication/321144770>.
26. Rojas LBA and Gomes MB: Metformin: an old but still the best treatment for type 2 diabetes. *Diabetology & Metabolic Syndrome* 2013; 5: 1-15.
27. Triggie C R, Mohammed I, Bshesh K, Marei I, Ye K, Ding H and Hill MA: Metformin: Is it a drug for all reasons and diseases?. *Metabolism* 2022; 133: 155223.
28. Petrie JR: Metformin beyond type 2 diabetes: Emerging and potential new indications. *Diabetes, Obesity and Metabolism* 2024; 26: 31-41. <https://doi.org/10.1111/dom.15756>.
29. Feng J, Wang X, Ye X, Ares I, Lopez-Torres B, Martínez M and Martínez MA: Mitochondria as an important target of metformin: The mechanism of action, toxic and side effects, and new therapeutic applications. *Pharmacology Research* 2022; 177: 106114. <https://doi.org/10.1016/j.phrs.2022.106114>.
30. Moussa AM, Sallam AM, Alamri HA, Alghamdi JA, Almohusseini NS, Alshahrani SM and Ali NSM: Study on the side effects and complications of metformin on diabetic patients. *International Journal of Pharmaceutical and Phytopharmacological Research* 2021; 11: 28-33. <https://doi.org/10.51847/eudg619>.
31. Brand-Williams W, Cuvelier ME and Berset C: Use of a free radical method to evaluate antioxidant activity. *Food Science Technology* 1995; 28(1): 25-30. [https://doi.org/10.1016/S0023-6438\(95\)80008-5](https://doi.org/10.1016/S0023-6438(95)80008-5).
32. Gulcin İ: Antioxidants and antioxidant methods: an updated overview. *Archives of Toxicology* 2020; 94(3): 651-715. <https://doi.org/10.1007/s00204-020-02689-3>.
33. Sarikurcu C, Sabih Ozer M, Cakir A, Eskici M and Mete E: GC/MS evaluation and *in-vitro* antioxidant activity of essential oil and solvent extracts of an endemic plant used as folk remedy in Turkey: *Phlomis bourgaei* Boiss. *Evidence-Based Complementary and Alternative Medicine* 2013; (1): 293080. <https://doi.org/10.1155/2013/293080>.
34. Verma VK, Prakash O, Kumar RSR, Rani KV *Phlomisbourgaei* Sehgal N: Water hyacinth (*Eichhornia crassipes*) leaves enhance disease resistance in *Channa punctata* from *Vibrio harveyi* infection. *The Journal of Basic and Applied Zoology* 2021; 82: 1-11. <https://doi.org/10.1186/s41936-020-00203-w>.
35. Alara OR, Abdurahman NH *Phlomisbourgaei* Ukaegbu CI: Extraction of phenolic compounds: A review. *Food Science* 2021; (4): 200-214. <https://doi.org/10.1016/j.cfrs.2021.03.011>.
36. Hoseinifar SH, Yousefi S, Van Doan H, Ashouri G, Gioacchini G, Maradonna, F and Carnevali O: Oxidative Stress and Antioxidant Defense in Fish: The Implications of Probiotic, Prebiotic, and Synbiotics 2020; 29(2): 198-217. <https://doi.org/10.1080/23308249.2020.1795616>.
37. Gedikoğlu A, Sökmen M and Çivit A: Evaluation of *Thymus vulgaris* and *Thymbra spicata* essential oils and plant extracts for chemical composition, antioxidant, and antimicrobial properties. *Food Science Nutrition* 2019; 7: 1704-1714. <https://doi.org/10.1002/fsn3.1007>.
38. Dangana RS, George RC and Agboola FK: The biosynthesis of zinc oxide nanoparticles using aqueous leaf extracts of *Cnidocolus aconitifolius* and their biological activities. *Green Chemistry Letters and Reviews* 2023; 16: 2169591. <https://doi.org/10.1080/17518253.2023.2169591>.

39. Gulcin İ and Alwasel SH: DPPH Radical Scavenging Assay. *Processes* 2023; 11(8): 2248. <https://doi.org/10.3390/pr11082248>.
40. Benabdallah A, Boumendjel M, Aissi O, Rahmoune C, Boussaid M and Messaoud C: Chemical composition, antioxidant activity and acetylcholinesterase inhibitory of wild *Mentha* species from northeastern Algeria. *South African Journal of Botany* 2018; 116: 131–139. <https://doi.org/10.1016/j.sajb.2018.03.002>.
41. Seleshe S, Ameer A and Kang SN: Exploration of the antioxidant chemical constituents and antioxidant performance of various solvent extracts of eighteen plants. *Preventive Nutrition and Food Science* 2022; 27: 212–222. <https://doi.org/10.3746/PNF.2022.27.2.212>.
42. Kwon JW, Lee HK, Park HJ, Kwon TO, Choi HR and Song JY: Screening of biological activities to different ethanol extracts of *Rubus coreanus* Miq. *Korean Journal of Medicinal Crop Science* 2011; 19(5): 325–333.
43. Naikoo MI, Dar MI, Raghib F, Jaleel H, Ahmad B, Raina A and Naushin F: Role and regulation of plants phenolics in abiotic stress tolerance: An overview. *Plant signaling molecules* 2019; 157–168. <https://doi.org/10.1016/B978-0-12-816451-8.00009-5>.
44. Sun W and Shahrajabian MH: Therapeutic potential of phenolic compounds in medicinal plants—Natural health products for human health. *Molecules* 2023; 28(4): 1845. <https://doi.org/10.3390/molecules28041845>.
45. Venkatesan T, Choi YW, Kim YK: Impact of different extraction solvents on phenolic content and antioxidant potential of *Pinus densiflora* bark extract. *BioMed Research International* 2019; (1): 3520675. <https://doi.org/10.1155/2019/3520675>.
46. Bhaktavalsala Suresh A and Kilingar Nadumane V: The metabolite 5-methyl-1, 3-benzenediol and its derivative methyl-2, 4-dihydroxy-6-methylbenzoate from the lichen *Parmotrema tinctorum* with potent apoptotic and anti-angiogenesis effects. *3 Biotechnol* 2021; 11(7): 346. <https://doi.org/10.1007/s13205-021-02883-9>.
47. Yuvaraj R, Rao MRK, Prabhu K, Sundram RL, Shil S, Kumar MS and Vijayalakshmi N: The gas chromatography–mass spectrometry study of one medicinal plant, *Stachytarpheta indica*. *Indian Journal of Pharmaceutical Science* 2019; 12(8): 382–394. <https://www.researchgate.net/publication/335618870>.
48. Takao K, Suzuki M, Miyazaki R, Miyake M, Akimitsu K and Hoshino K: Immunomodulatory effects of D-allose on cytokine production by plasmacytoid dendritic cells. *Biochemical and Biophysical Research Communications* 2022; 627: 130–136. <https://doi.org/10.1016/j.bbrc.2022.08.037>.
49. Tohi Y, Taoka R, Zhang X, Matsuoka Y, Yoshihara A, Ibuki E and Sugimoto M: Antitumor effects of orally administered rare sugar D-allose in bladder cancer. *International Journal of Molecular Sciences* 2022; 23(12): 6771. <https://doi.org/10.3390/ijms23126771>.
50. Fadipe LA, Haruna AK and Mohammed I: Antibacterial activity of 1, 2-benzenedicarboxylic acid, dioctyl ester isolated from the ethyl acetate soluble sub-portion of the unripe fruits of *Nauclea latifolia* 2014. [www.ijpab.com](http://www.ijpab.com).
51. Okechukwu PN: Evaluation of anti-inflammatory, analgesic, antipyretic effect of eicosane, pentadecane, octacosane, and heneicosane. *Asian Journal of Pharmaceutical and Clinical Research* 2020; 13(4). <https://doi.org/10.22159/ajpcr.2020.v13i4.36196>.
52. Arumugam M, Manikandan DB, Sridhar A, Palaniyappan S, Jayaraman S and Ramasamy T: GC–MS Based Metabolomics strategy for cost-effective valorization of Agricultural Waste: Groundnut Shell Extracts and Their Biological Inhibitory Potential. *Waste Biomass Valorization* 2022; 13(10): 4179–4209. <https://doi.org/10.1007/s12649-022-01768-z>.
53. Arora S and Saini M: Gas chromatography mass spectrometry profiling in methanolic and ethyl-acetate root and stem extract of *Corbichonia decumbens* (Forssk.) exell from Thar Desert of Rajasthan, India. *Pharmacognosy Research* 2017; 9: 48–52. [https://doi.org/10.4103/pr.pr\\_62\\_17](https://doi.org/10.4103/pr.pr_62_17).
54. Juárez-Rodríguez M M, Cortes-López H, García-Contreras R, González-Pedrajo B, Díaz-Guerrero M, Martínez-Vázquez M and Castillo-Juárez I: Tetradecanoic acids with anti-virulence properties increase the pathogenicity of *Pseudomonas aeruginosa* in a murine cutaneous infection model. *Frontiers in Cellular and Infection Microbiology* 2021; 10: 597517. <https://doi.org/10.3389/fcimb.2020.597517>.
55. Bhardwaj M, Sali V K, Mani S and Vasanthi HR: Neophytadiene from *Turbinaria ornata* suppresses LPS-induced inflammatory response in RAW 264.7 macrophages and Sprague Dawley rats. *Inflammation* 2020; 43: 937–950. <https://doi.org/10.1007/s10753-020-01179-z>.
56. Ibrahim H, Uttu AJ, Sallau MS and Iyun ORA: Gas chromatography–mass spectrometry (GC–MS) analysis of ethyl acetate root bark extract of *Strychnos innocua* (Delile). *Beni-Suef University Journal of Basic and Applied Sciences* 2021; 10: 1–8. <https://doi.org/10.1186/s43088-021-00156-1>.
57. Yang M, Li XL, Wang JR, Lei X, Tang W, Li XW and Guo YW: Sarcomililite A, an unusual diterpenoid with tricyclo 11.3. 0.02, 16hexadecane carbonskeleton and its potential biogenetic precursors from the Hainan soft coral *Sarcophyton mililatensis*. *The Journal of Organic Chemistry* 2019; 84: 2568–2576. <https://doi.org/10.1021/acs.joc.8b03020>.
58. Chen ZH, Li WS, Zhang ZY, Luo H, Wang JR, Zhang HY and Guo YW: Sinusiaetone A, an Anti-inflammatory Norditerpenoid with a Bicyclo11.3.0hexadecane Nucleus from the Hainan Soft Coral *Sinularia siaesensis*. *Organic letters* 2021; 23(15): 5621–5625. <https://doi.org/10.1021/acs.orglett.1c01601>.
59. Huang L, Zhu X, Zhou S, Cheng Z, Shi K, Zhang C and Shao H: Phthalic acid esters: Natural sources and biological activities. *Toxins* 2021; 13(7): 495. <https://doi.org/10.3390/toxins13070495>.
60. Deepa PK, Subramanian A and Manjusha WA: Evaluation of antioxidant potential and bioactive metabolites of *Nanno chloropsis* sp. *Journal of Advanced Applied Scientific Research* 2020; 2(5): 1–9.
61. Ganesan T, Subban M, Christopher Leslee DB, Kuppannan S B and Seedeve P: Structural characterization of n-hexadecanoic acid from the leaves of *Ipomoea eriocarpa* and its antioxidant and antibacterial activities. *Biomass Conversion and Biorefinery* 2022; 14(13): 14547–14558. <https://doi.org/10.1007/s13399-022-03576-w>.
62. Tassakka ACMA, Sumule O, Massi MN, Manggau M, Iskandar IW, Alam JF and Liao LM: Potential bioactive compounds as SARS-CoV-2 inhibitors from extracts of the marine red alga *Halymenia durvillei* (Rhodophyta)—A computational study *Arabian Journal of Chemistry* 2021; 14(11): 103393. <https://doi.org/10.1016/j.arabjc.2021.103393>.
63. An K, Fu M, Zhang H, Tang D, Xu Y and Xiao G: Effect of ethyl oleate pretreatment on blueberry (*Vaccinium corymbosum* L.): drying kinetics, antioxidant activity, and

- structure of wax layer. Journal of Food Science and Technology 2019; 56(2): 783-791.
64. Abcha I, Souilem S, Neves M A, Wang Z and Nefatti M: Ethyl oleate food-grade O/W emulsions loaded with apigenin: Insights to their formulation characteristics and physico-chemical stability. Food Research International 2019; 116: 953-962. <https://doi.org/10.1016/j.foodres.2018.09.032>.
  65. Ita BN and Ngochindo RI: Novel Compounds from *Homalium letestui* (Flacourtiaceae). Journal of Chemical Society of Nigeria 2019; 44(2).
  66. Bekiesch P, Zehl M, Domingo-Contreras E, Martín J, Pérez-Victoria I, Reyes F and Zotchev SB: Viennamycins: Lipopeptides produced by a *Streptomyces* sp. Journal of Natural Products 2020; 83(8): 2381-2389. <https://doi.org/10.1021/acs.jnatprod.0c00152>.
  67. Charles JI and Minakiri IS: Evaluation of the Antibacterial Activity of *Chromolaena Odorata* in Wistar Rats and its Chemical Characterization. Technology, and Sciences (ASRJETS) American Scientific Research Journal for Engineering 2018; 42: 111-129. <http://asrjetsjournal.org/>
  68. Ahsan T, Chen J, Zhao X, Irfan M, Wu Y: Extraction, and identification of bioactive compounds (eicosane and dibutyl phthalate) produced by *Streptomyces* strain KX852460 for the biological control of *Rhizoctonia solani* AG-3 strain KX852461 to control target spot disease in tobacco leaf. AMB Express 2017; 7: 1-9. <https://doi.org/10.1186/s13568-017-0351-z>.
  69. Mamedov IG, Shikhaliyeva IM, Mamedova YV, Abdurahmanli SG and Maharramov AM: Antibacterial and antifungal activities of thiosemicarbazone, pyrazole, indole, cyclohexanol derivatives of 2-hydroxy-5-methyl- and 4-bromoacetophenones. Indian Journal of Chemistry 2019; 58. <http://nopr.niscpr.res.in/handle/123456789/49791>.
  70. Akkoyunlu A and Dulger G: Chemical Composition of *Lamium purpureum* L. and Determination of Anticancer Activity of Its Essential Oil on Melanoma. Düzce Üniversitesi Bilim ve Teknoloji Dergisi 2019; 7: 1755-1763. <https://doi.org/10.29130/dubited.553793>.
  71. *Moringa oleifera* Leaves of Kolli Hills at Namakkal against Colorectal Cancer Venkatachalam Bharathi Vivekanandha Educational Institutions, (n.d.).
  72. Aadesariya MK, Ram VR and Dave PN: Phytochemical Analysis of leaves Extract of *Abutilon pannosuminn-Butanol* for its Bioactive Components through Gas Chromatography-Mass Spectrometry (GC-MS). Phytochemical Analysis 2018; 8(9).
  73. Szymański M, Dudek-Makuch M, Witkowska-Banaszczak E, Bylka W and Szymański A: Comparison of the Chemical Composition and Antioxidant Activity of Essential Oils from the Leaves and Flowers of *Sambucus nigra*. Pharmaceutical Chemistry Journal 2020; 54: 496-503. <https://doi.org/10.1007/s11094-020-02228-5>.
  74. Muniyan R, Sundararajan S and Jochebed JS: Antimicrobial and Antimycobacterial properties of *Solanum trilobatum* L.-in-vitro. Research Journal of Pharmacy and Technology 2022; 15: 5603-5609. <https://doi.org/10.52711/0974-360X.2022.00946>.
  75. Uddin MZ, Paul A, Rakib A, Sami SA, Mahmud S, Rana MS and Simal-Gandara J: Chemical profiles and pharmacological properties with *in-silico* studies on *Elatostema papillosumwedd*. Molecules 2021; 26(4): 809. <https://doi.org/10.3390/molecules26040809>.
  76. Nazir S, Chaudhary W A, Mobashar A, Anjum I, Hameed S and Azhar S: Campesterol: a natural phytochemical with anti inflammatory properties as potential therapeutic agent for rheumatoid arthritis: a systematic review. Pakistan Journal of Health Sciences 2023; <https://doi.org/10.54393/pjhs.v4i05.792>.
  77. Hanafy RS and Sadak MS: Foliar spray of stigmasterol regulates physiological processes and antioxidant mechanisms to improve yield and quality of sunflower under drought stress. Journal of Soil Science and Plant Nutrition 2023; 23: 2433-2450. <https://doi.org/10.1007/s42729-023-01197-4>.
  78. Jiao Y, Shi C and Sun Y: (2023). Unravelling the Role of *Scutellaria baicalensis* for the Treatment of Breast Cancer Using Network Pharmacology, Molecular Docking, and Molecular Dynamics Simulation. International Journal of Molecular Sciences 2023; 24(12): 10370. <https://doi.org/10.3390/ijms24043594>.
  79. Wang H, Wang Z, Zhang Z, Liu J and Hong L:  $\beta$ -Sitosterol as a promising anticancer agent for chemoprevention and chemotherapy: mechanisms of action and future prospects. Advances in Nutrition 2023; 14(5): 1085-1110. <https://doi.org/10.1016/j.advnut.2023.05.013>
  80. Khan Z, Nath N, Rauf A, Emran T B, Mitra S, Islam F and Thiruvengadam M: Multifunctional roles and pharmacological potential of  $\beta$ -sitosterol: Emerging evidence toward clinical applications. Chemico-biological Interactions 2022; 365: 110117. <https://doi.org/10.1016/j.cbi.2022.110117>.
  81. Thirumalaisamy R, Ameen F, Subramanian A, Selvankumar T, Alwakeel SS and Govarthanan M: *In-vitro* and *in-silico* Anti-inflammatory Activity of Lupeol Isolated from *Crateva adansonii* and Its Hidden Molecular Mechanism, International Journal of Peptide Research and Therapeutics. 2020; 26: 2179-2189. <https://doi.org/10.1007/s10989-019-10006-5>.
  82. Liu K, Zhang X, Xie L, Deng M and Chen H: Lupeol and its derivatives as anticancer and anti-inflammatory agents: Molecular mechanisms and therapeutic efficacy. Pharmacological Research 2021; 164: 105373. <https://doi.org/10.1016/j.phrs.2020.105373>.
  83. Li D, Guo YY, Cen X F, Qiu H L, Chen S, Zeng XF and Tang QZ: Lupeol protects against cardiac hypertrophy via TLR4-PI3K-Akt-NF- $\kappa$ B pathways. Acta Pharmacologica Sinica 2022; 43: 1989-2002. <https://doi.org/10.1038/s41401-021-00820-3>.

**How to cite this article:**

Rani S, Verma VK, Sehgal N and Prakash O: *In-vitro* and *in-silico* study of *Butea monosperma* flower. Int J Pharm Sci & Res 2025; 16(10): 2783-93. doi: 10.13040/IJPSR.0975-8232.16(10).2783-93.

All © 2025 are reserved by International Journal of Pharmaceutical Sciences and Research. This Journal licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported License.

This article can be downloaded to **Android OS** based mobile. Scan QR Code using Code/Bar Scanner from your mobile. (Scanners are available on Google Playstore)