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Chemical Constitution, *In-silico* Molecular Docking Studies and Antibacterial Activity of Flower Essential Oil of *Artabotrys hexapetalus*

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ABSTRACT

The isolation of the volatile constituents from the flowers of *Artabotrys hexapetalus* was carried out using a simple headspace solvent-trapping technique and identified by GC-MS analysis. The major compounds are ethyl acetate 53.6%, isobutyl acetate (29.4%) and ethyl benzoate (14.2%). The odour of the solution obtained from this method was found to be similar to that of the fresh flowers. Further the essential oil from *A. hexapetalus* was obtained for the first time from India by hydro distillation using a Clevenger type apparatus and analysed by GC-MS. The plant yielded 1.26%, of the essential oils from the flower. The analysis lead to the identification of 28 compounds representing 96.17% of the total oil. The essential oil consists of predominantly oxygenated sesquiterpenes (51.91%) followed by sesquiterpenes (43.31%) and small quantities of monoterpenes (1.24%) and other compounds (1.34%). The main constituents of the essential oil obtained from the flowers of *A.hexapetalus* are β-caryophyllene (18.69%), caryophyllene oxide (14.54%), cubenol (12.53%) and ledol (11.5%). The essential oil showed antibacterial activity against bacterial strains *Streptococcus pneumonia*, *Staphylococcus aureus*, *Streptococcus pyogenes* and *Pseudomonas aeruginosa* exhibiting a zone of inhibition of 16.4, 15.7, 17.5 and 14.5 mm and MIC value of 2.5, 5.0, 2.5, 5.0 mg/ml respectively. Molecular docking analysis indicated that the essential oil constituents are nucleic acid and cell wall synthesis inhibitors. So it is worth to include this in cosmetics and fragrances.

Keywords: *Artabotrys hexapetalus*, essential oil, GC-MS, sesquiterpenes, β-caryophyllene, antibacterial, docking.

1. INTRODUCTION

Artabotrys species are traditionally used for a wide range of diseases like cholera, scrofula and malaria. The fruits and leaves of *Artabotrys* species are utilized as animal feeds, predominantly for goats, chimpanzees and cattle [1]. Due to the fragrance of the flowers of *Artabotrys* species, they are used as flavouring agents, in the manufacture of perfumes and for making stimulating tea-like beverages. Boiled juice of flowers is a stimulating beverage and used to treat vomiting, biliousness, blood diseases, heart and bladder disorders, itching and leucoderma[2]. They are used in the treatment of bad breath, headache, sweating, and thirst and also used as cardiotonic[3,4]. *A. hehapetalus* has numerous activities such as antispermatogenic, antiandrogenic, antioxidant, antimicrobial, and antidenaturation of protein, antiproteinase and anti-inflammatory.

The flowers from *A. hexapetalus* (Fig 1) have a sweet and fresh odour and however it was investigated only once from Thailand[5] to identify the volatile compounds responsible for its odour and from Vietnam to study the chemical composition of the essential oil[6]. To our knowledge we are investigating for the first time to identify these compounds from India. The sweet and fresh smell from this flower comes only between 5 to 8 a.m. in the morning and 6 to 8 p.m. in the evening[5]. It means that the compounds responsible for this odour from the flower are

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released only within this period of time. Therefore, it is important that the onsite sampling and preconcentration steps are to be focussed in order to identify the volatile constituents of the flowers from *A. hexapetalus*. Thus the objective of the present work is to identify the chemical composition of the essential oil from flowers of *A. hexapetalus* after giving due importance to the onsite sampling and precondition step. Further another objective of the present work is to investigate the antimicrobial activity of the essential oil obtained from *A. hexapetalus* and to find a mechanism of the action of antimicrobial activity by molecular docking study. Several drugs that are currently available to the public for the treatment of different diseases have been developed based on in silico approaches. For example, Zanamivir, used to treat influenza, was developed using computer-assisted design[7] [A]. Nelfinavir and Saquinavar are used in the treatment of HIV and were also developed by computational methods[8]. [B].

Fig.1. Flower from *A. hexapetalus*

2. Materials and Methods

2.1. Plant Material

The flower of *A. hexapetalus* were collected (200 g) from the Coimbatore District (coordinates: 10.9880° N, 76.7740° E), Tamilnadu, India between 6 to 7 a.m. in the morning during the month of January 2018. The plant material was authenticated by Dr. R. Gopalan, Professor of Botany Department, KAHE, Coimbatore (Voucher No. KAHE/CHE/2018/102).

2.2. Extraction of Essential Oil

After the onsite collection of the flowers between 6 to 7 a.m. in the morning the components were extracted immediately using a simple head space-solvent technique. In this method about 500 g of the flower were taken in an Erlenmeyer flask (500 ml capacity) fitted with a one holed rubber cork. Using an aquarium pump fresh air was blown in continuously through the inlet of the flask for nine hours. The vapour collected on the top surface of the flask was allowed to pass in to a round bottomed flask having 30 ml of methylene chloride solvent. This was repeated four times and the combined resulting solution was concentrated to 2 ml in a rotary evaporator and the concentrate was analysed by GC-MS.

Fresh flowers obtained (500 g) were chopped into small pieces and subjected to hydro distillation. A quantity of 60 g of the flowers *A. hexapetalus* was added to 300 ml of distilled water in a one litre flask fitted with a Clevenger apparatus and a condenser through which cold water was circulated to ensure condensation of essential oils for 2 h. This was repeated twice. At the end of the distillation, two phases were observed, an organic phase (essential oil) and an aqueous phase (aromatic water). The essential oil was collected, dried under anhydrous sodium sulphate. Until further analysis the resulted oil was stored at 4°C in a refrigerator.

2.3. Determination of Chemical Composition of Essential Oil

GC-MS along with an ESI system with the ionization energy of 70 eV was utilized for essential oil composition

analysis. Agilent Technologies, 7890A, with a HP-5MS column (5 % phenyl methylpolysiloxane) 30 m × 0.25 mm ID × 0.25 μm film. The mass spectrometer with an ion-trap analyzer was set at 1508 for all analyses with an electron multiplier voltage of 1058V. Scanning was performed from m/z 39 to 400 in 70 eV EI (electronic impact) at 1 scan/ s-1 and the selected split ratio was 1:10. Helium (99.99%) with the flow rate of 1ml/min was used as the carrier gas. The injection part of the instrument was set at a temperature of 250ºC. The initial temperature of the column was maintained at 40°C for 1min, and then gradually increased to 240ºC at the rate of 30ºC/min. Essential oil constituents were tentatively identified by comparison of their GC retention indices (RI), determined with reference to a homologous series of C8-C20 n-alkanes and with those of available authentic standards and literature. Confirmation of such identification was done by comparing their mass spectral fragmentation patterns with those stored in the MS database (NIST 2005 and Wiley 7N libraries) and with mass spectra literature data. Components relative concentrations were obtained with the response factors to the FID.

2.4. Antibacterial screening

The antibacterial screening by zone of inhibition method and determination of Minimum inhibitory concentration (MIC) were determined using the bacterial strains like *Streptococcus pneumonia*, *Staphylococcus aureus*, *Streptococcus pyogenes* and *Pseudomonas aeruginosa* by the method as we reported earlier[9].

2.5. Molecular Docking

2.5.1. Preparation of Proteins and ligands

The three-dimensional structure of the proteins with PDB id: 3UDI, 3TYE, 3TTZ and 1JZQ were downloaded from the RCSB protein Data Bank and saved in PDB file format, for further studies in Auto dock vina under PyRx 0.8 Platform.

The compounds present in the essential oil obtained from *A. hexapetalus* were selected for docking studies. Molecular docking study has been carried out using the PyRx Version 0.8 docking program. Ligands 2D structures were drawn and converted into 3D using Chem Office 2002. After energy minimization of the ligands, it was docked with the protein's target sites (amino acids). Discovery studio was used to convert 2D in to 3D structure and the energy was minimized using AM1 method. To minimise the energy to minimum RMS gradient of 0.100 was set in each interaction. All structures were saved as PDB file format. All the ligand structures were then saved in SDF file format, to carry out docking in Autodock vina[10]. A grid box with dimension of 40 x 40 x 40A with 0.37A spacing and cantered on 29.47, 47.99, 8.86 was created around the binding site on proteins. The centre of the box was set a ligand centre, and grid energy calculations were carried out.

3. Results and Discussion

The isolation of the volatile constituents from the flowers of *A. hexapetalus* was carried out using a simple headspace solvent-trapping technique and the headspace vapour was flushed with air and collected in solvent methylene chloride. When analysed by GC-MS, Six compounds were identified from the resultant concentrated methylene chloride solution. The identified volatile compounds are ethyl acetate 53.6%, isobutyl acetate (29.4%) and ethyl benzoate (14.2%) as major compounds and ethyl propionate (1.6%), ethyl octonate (0.7%) and isobutyl valerate (0.43%) as minor compounds. The odour of the solution obtained from this method was identified to be similar to that of the fresh flowers. The presence of ethyl benzoate and ethyl propionate in the present investigation of the volatile constituents from the flowers of *A. hexapetalus* make the smell of the flowers of *A. hexapetalus* from India different from the flowers of *A. hexapetalus* from Thailand[5].

The chromatogram obtained from the GC-MS analyses was shown in Figure 2. It resulted in the identification of 28 compounds (Figure 3) representing 96.17% of the oil. The plant yielded 0.36%, (0.68 g) of the essential oils from the flower (the average yield of three

distillations). The essential oil consists of predominantly oxygenated sesquiterpenes (51.91%) followed by sesquiterpenes (43.31%), monoterpenes (1.24%) and small quantities of other compounds (1.82%). The GC-MS analysis results are summarized in the Table 1. Caryophyllene oxide (14.54%), β-caryophyllene (18.69%), cubenol (12.53%) and ledol (11.5%) were the main constituents of the essential oil of the flowers. It is having a strong green odour and differs a lot from the smell of the fresh flowers. This is due to the reason that in the high temperature prevailed during the hydrodistillation, the enzymatic processes that were responsible for the odour formation and release of the compounds would have denatured[11]. Hence the compounds which contribute to the significance odour could not be accumulated in the obtained essential oil.

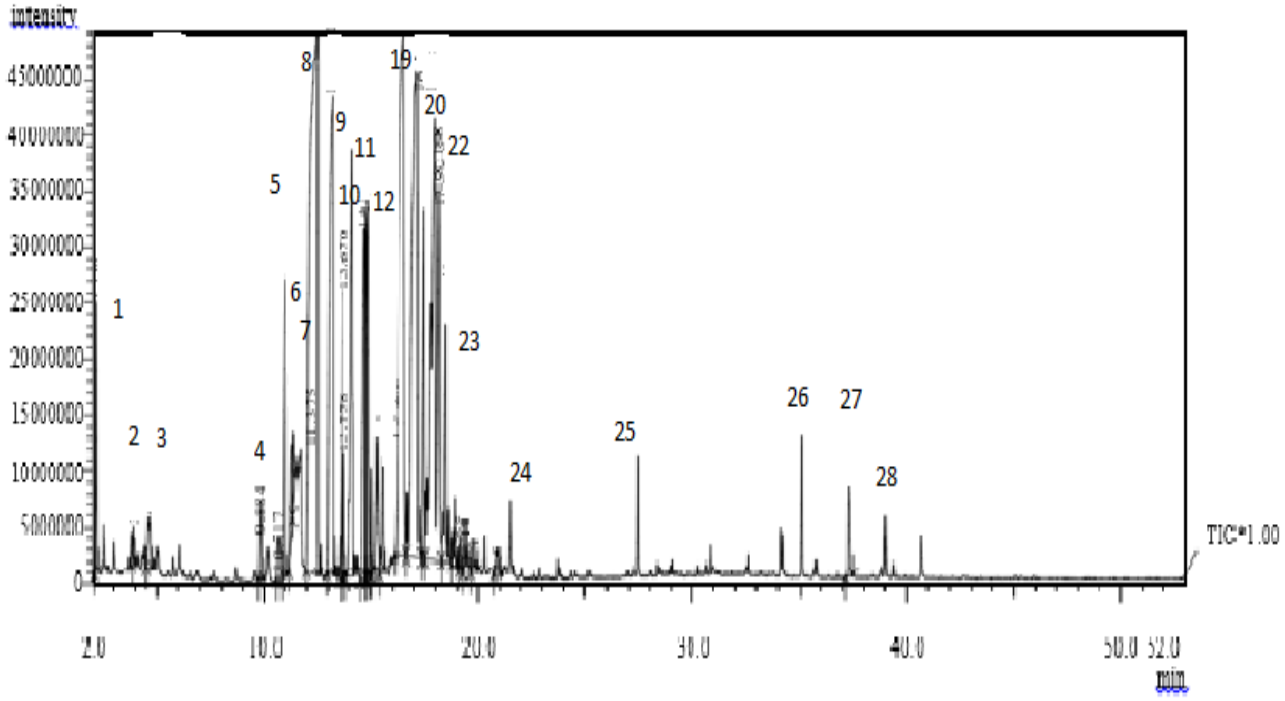

Figure 2: GC-MS Chromatogram of essential oil obtained from *A. hexapetalus*.

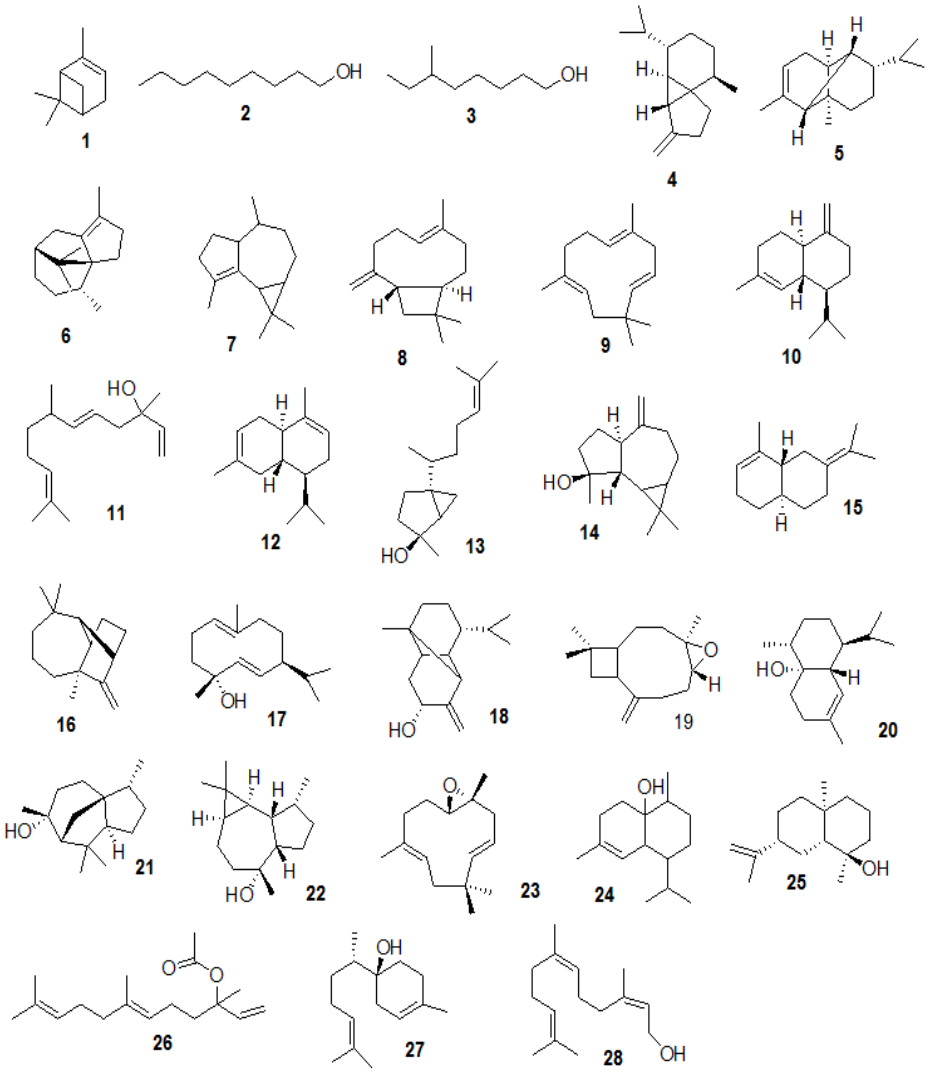

Fig. 3 Structure of the compounds identified from the essential oil from the flowers of *A. hexapetalus*

In an earlier study twenty-eight components comprising of sesquiterpenes hydrocarbons (33% of the oil) and oxygenated sesquiterpenes (47.7%) were reported from the flower oil of *A. hexapetalus* collected from Vietnam. The major compounds are α-copaene (8.1%), β-elemene (1.0%), β-caryophyllene (11.4%), α-humulene (3.5%), γ-muurolene (3.5%), caryophyllene oxide (31.5%), and humulene epoxide (10.01%) [12].

Table 1. Essential oil composition of *Artabotrys hexapetalus* as determined by GC-MS

Compound.No	Retention time[a]	Compound[b,c]	%[d]	Molecules formulae	Retention Index[e]
1	2.1	α-pinene	1.24	$C_{10}H_{16}$	934
2	3.94	1-Nonanol	0.20	$C_9H_{20}O$	1089
3	4.68	6-Methyloctan-1-ol	0.64	$C_9H_{20}O$	1109
4	10.71	β-Cubeben	0.41	$C_{15}H_{24}$	1333
5	11.013	Copaene	3.91	$C_{15}H_{26}$	1375
6	11.375	cyperene	1.00	$C_{15}H_{24}$	1398
7	11.452	α -Gurjunene	0.59	$C_{15}H_{24}$	1405
8	12.53	β-Caryophyllene	18.67	$C_{15}H_{24}$	1420
9	13.263	Humulene	8.24	$C_{15}H_{24}$	1449
10	13.670	γ-cadinene	1.97	$C_{15}H_{24}$	1505
11	13.778	Nerolidol	0.60	$C_{15}H_{26}O$	1520
12	14.19	β-cadinene	4.88	$C_{15}H_{24}$	1530
13	14.70	Sesquisabinene Hydrate	3.86	$C_{15}H_{26}O$	1534
14	14.79	Spathulanol	2.29	$C_{15}H_{26}O$	1566
15	14.97	Selina-3,7 (11)-diene	3.18	$C_{15}H_{24}$	1567
16	14.98	Longifolene	0.21	$C_{15}H_{24}$	1568
17	15.067	Germacrene D-4-ol	0.46	$C_{15}H_{26}O$	1569
18	15.29	β-Copaene-4α-ol	1.16	$C_{15}H_{26}O$	1570
19	16.58	Carryophyllene oxide	13.46	$C_{15}H_{26}O$	1573
20	17.18	Cubenol	12.53	$C_{15}H_{26}O$	1590
21	17.52	cedrol	2.49	$C_{15}H_{26}O$	1592
22	18.14	Ledol	11.57	$C_{15}H_{26}O$	1594
23	18.51	Humulene epoxide	2.18	$C_{15}H_{26}O$	1597
24	21.42	1-Cubenol, epi	0.58	$C_{15}H_{26}O$	1614
25	27.12	Selin-11-en-4α-ol	0.25	$C_{15}H_{24}$	1641
26	35.04	Nerolidol-Epoxyacetate	0.50	$C_{17}H_{28}O_2$	1687
27	37.21	β-Bisabolol	0.41	$C_{15}H_{26}O$	1689
28	39.06	Farnesol	0.32	$C_{15}H_{26}O$	1733

[a]Compounds are listed in order of their elution from a HP-5MS column.

[b]Identification: MS, based on comparison with NIST 14 MS databases;

[c]Retention index from NIST 14 and Wiley 275 mass spectral databases.

[d]Quantification was done by external standard method using calibration curves generated by running GC analysis of representative authentic components

[e]Retention index on the HP-5MS column, calculated using homologous series of C_9–C_{18} alkanes.

From Thailand the essential oil was obtained by four different process like simple headspace solvent-trapping technique, solvent extraction, hydro distillation, and solid phase micro extraction (SPME) and the identified compounds were reported[5]. Oil from the hydro distillation method showed the presence of thirty one components, of which the major components were β-gurjunene (30.0%), Globulol (13.8%) and β-caryophyllene (10.1%). Essential oil obtained from the same source by solvent extraction led to the identification of thirty one components of which the major compounds were isopentyl acetate (12.6%), linalool (7.7%), 2-methylbutyl acetate (7.7%), limonene (5.7%) and 3-methylbutanol (5.7%). Alternatively when it was performed with solid-phase micro extraction (SPME) methods, thirty nine components were identified with ethyl acetate (12.8%) and isobutyl acetate (39.5%) as the major components[5]. Further Cadinol, spathulenol, β-caryophyllene oxide and cubenol (-) were reported from the essential oil obtained from Tanzania. The volatile constituents are dominated by sesquiterpene hydrocarbons and oxygenated sesquiterpenoids[14].

The present study showed that the chemical constituents from the essential obtained from Indian *A. hexapetalus* are found to be different with the essential oil obtained by the hydro distillation method from Tanzania[13] and Vietnam[12] and Thailand. In our study the quantity of β-caryophyllene is more than the caryophyllene oxide where as in the above studies caryophyllene oxide is more than that of β-caryophyllene. The study indicated that the sesquiterpenes β-caryophyllene oxide to be present in almost all essential oils obtained by hydro distillation of the *A. hexapetalus*. β-caryophyllene oxide was reported to exhibit mosquito repellent activity.

3.1. Antibacterial Screening

The diameter of zone of inhibition was measured in mm and presented in the table 2. The essential oil from *A. hexapetalus* exhibited inhibitory activity against all the bacterial strains *Streptococcus pneumonia, Staphylococcus aureus, Streptococcus pyogenes* and *Pseudomonas aeruginosa* with MIC values of 2.5, 5.0, 2.5, 5.0 mg/ml and narrow inhibition zones of 16.4, 15.7, 17.5 and 14.5 mm respectively. Ampicillin was used as a positive control. Overall the results suggest that the essential oil of *A. hexapetalus* have a potential antibacterial activity. The activity is attributed to the various constituents present in the essential oil obtained from the flowers of *A. hexapetalus.*

3.2. Molecular Docking

Antibiotics may either kill or inhibit the growth of bacteria by different mechanisms[15,16]. Now, in the current study, the knowledge on the target proteins of currently used antibiotics[17,18] is extended to the phytoconstituents which is identified from *A. hexapetalus* in order to examine their affinity with the bacterial proteins that are well known targets for some antibiotics with different mechanism of action such as cell wall synthesis, inhibitors of nucleic acid synthesis and antimetabolites. In the present study we carriedout the molecular docking studies with 3UDI (acinetobacter baumannii in complex with penicillin G), 3TYE (dihydropteroate synthase), 3TTZ (DNA gyrase) and 1JZQ (Isoleucyl-tRNA synthetase) proteins which represent the above three mechanisms. The docking score of the ligands with the protein 3TTZ and 1JZQ are not encourageable and hence not pursued further.

One of the target protein (PDB id: 3UDI) is from murD ligase which is involved in the cell wall synthesis and the other target is dihydropteroate synthase enzyme (DHPS; PDB id: 3TYE) a key component in the folate pathway of bacteria and primitive eukaryotes. The essential oil constituents were docked against these two targets and the compounds with a reasonable docking score (Kcal/mole) are presented in the table 3. Most of the ligands exhibited hydrophobic interactions (Figure 4a-4d) with the target proteins which are evidenced by their docking scores. This indicates that the essential oil components of *A. hexapetalus* behave as inhibitors of nucleic acids and cell wall synthesis inhibitors which involve in cell well synthesis. So we hypothesise that these essential oil constituents first interact with the cell wall to destruct the cell structure and then inhibits the normal synthesis of DNA that are

required for bacterial growth. β-Lactams act entirely outside the cell membrane, in the final phase of peptidoglycan biosynthesis. Sulfonamides inhibit the action of dihydropteroate synthetase (with p-aminobenzoic acid (PABA) as substrate), preventing the synthesis of dihydrofolic acid[17,20]. So, from the present study we can say that these compounds act on the multi targets and may serve as antibacterial agents.

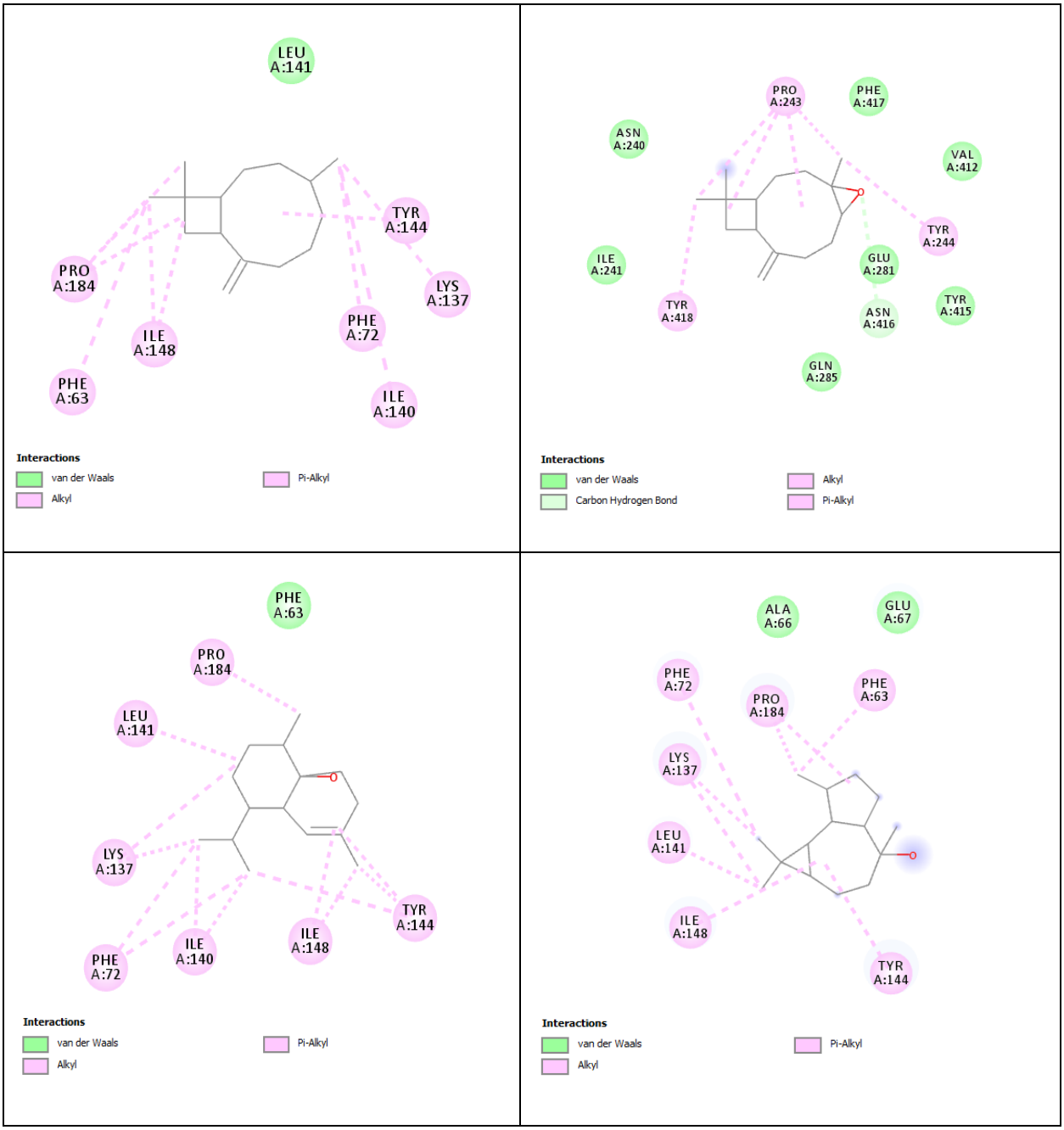

Figure 4a: Molecular docking of Trans (beta)-caryophyllene, caryophyllene oxide, Cubenol and Ledol against the target protein with the PDB id: 3UDI

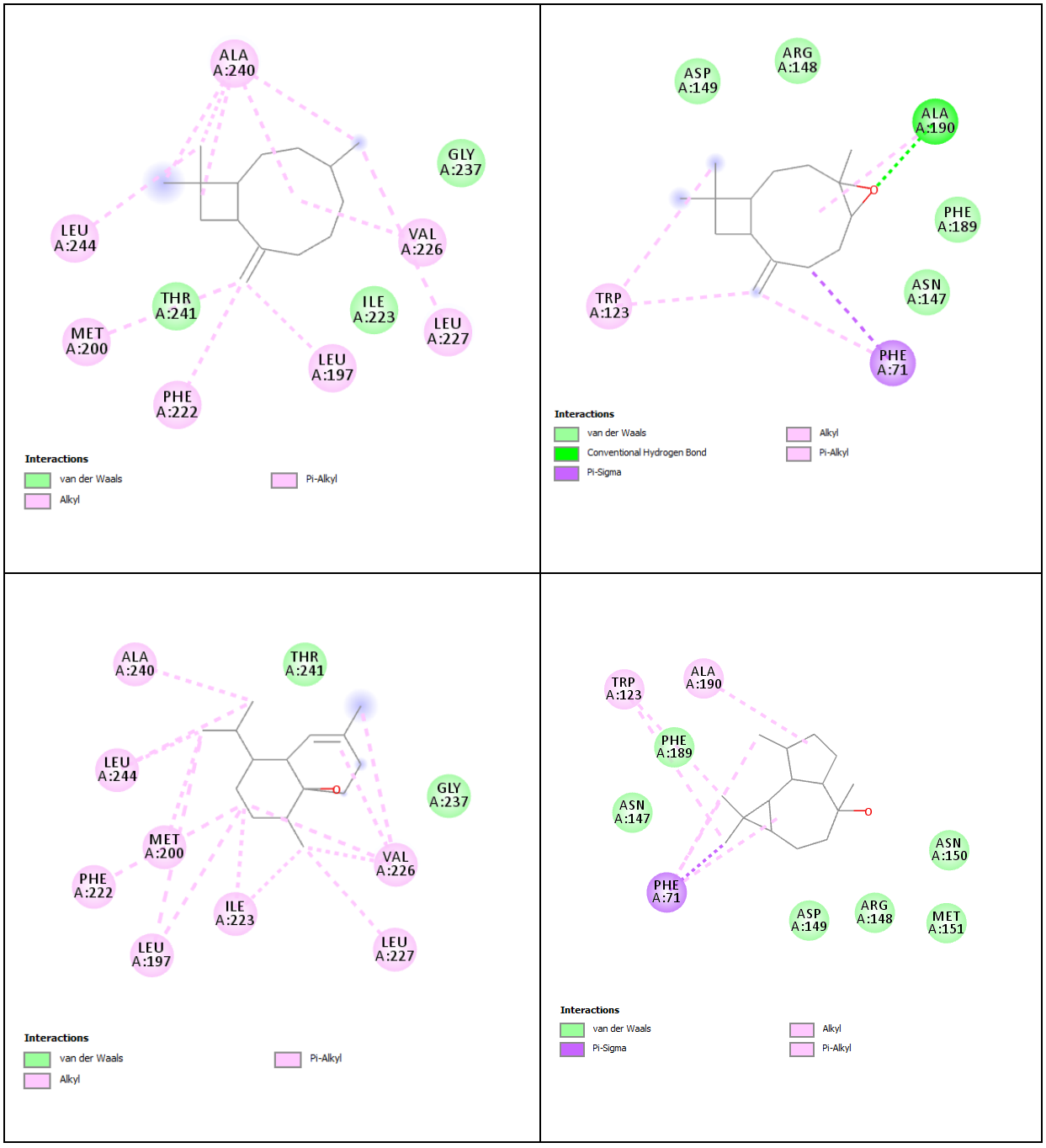

Figure 4b: Molecular docking of Trans (beta)-caryophyllene, caryophyllene oxide, Cubenol and Ledol against the target protein with the PDB id: 3TYE

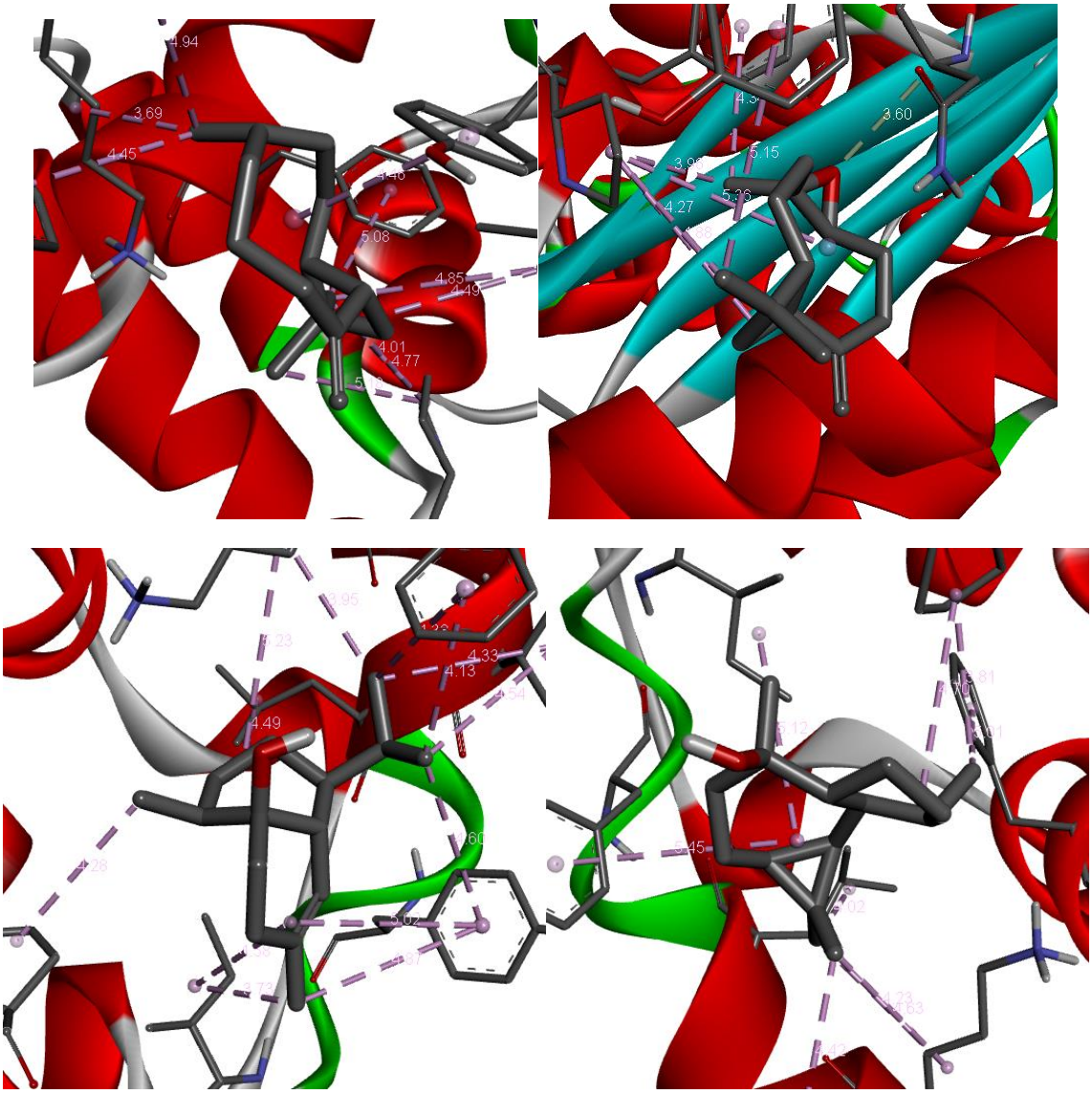

Figure 4c: Molecular docking 3D images of Trans (beta)-caryophyllene, caryophyllene oxide, Cubenol and Ledol against the target protein with the PDB id: 3UDI

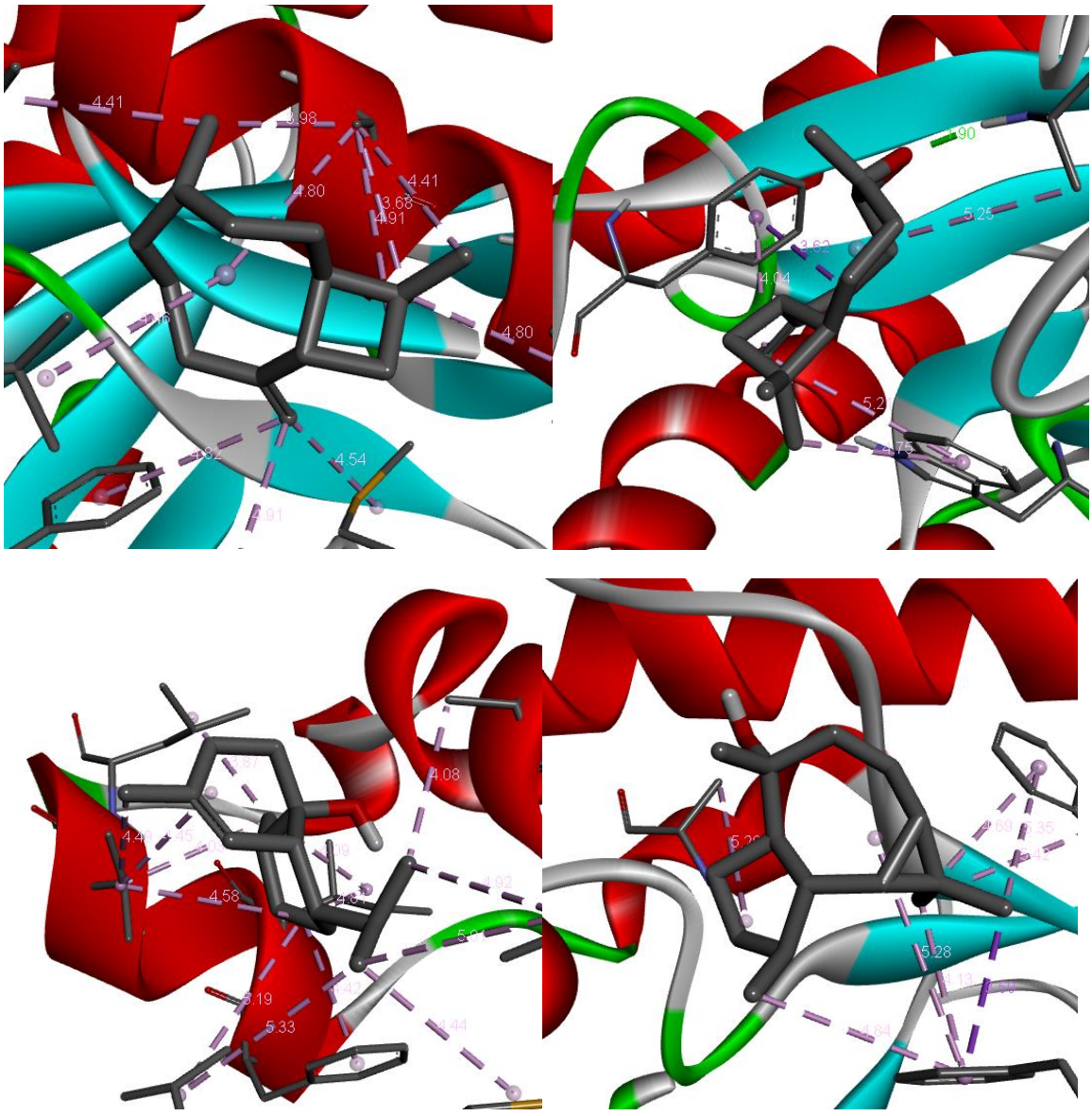

Figure 4d: Molecular docking 3D images of Trans (beta)-caryophyllene, caryophyllene oxide, Cubenol and Ledol against the target protein with the PDB id: 3TYE

Table 2. Antibacterial activity of the essential oil obtained from the flowers of *A. hexapetalus*

Bacterial strain	Zone of Inhibition(mm)		Minimum Inhibitory Concentration(mg)	
	Essential oil	Ampicillin	Essential oil	Ampicillin
Streptococcus pneumonia	16.4	19.5	2.5	2.5
Staphylococcus aureus	15.7	21.5	5.0	2.5
Streptococcus pyogenes	17.5	23.5	2.5	2.5
Pseudomonas aeruginosa	14.5	21.5	5.0	2.5

Table 3. Molecular docking analysis of the essential oil constituents from *A. hexapetalus* against bacterial proteins

Ligands	Docking score 3TYE (Kcal/mole)	Docking score 3UDI (Kcal/mole)
Trans(beta)-caryophyllene	-6.8	-6.9
Carryophyllene oxide	-6.4	-7.0
Cubenol	-6.0	-6.9
Ledol	-6.6	-6.8

4. Conclusion

Using the simple headspace solvent-trapping technique in association with GCMS the components responsible for the odour of the flowers of *A. hexapetalus* flowers were identified. The essential oil obtained from the flowers of *A. hexapetalus by* hydro distillation was analysed by GC-MS, and it lead to the identification of 28 compounds predominantly oxygenated sesquiterpenes (51.91%). Caryophyllene oxide (14.54%), β-caryophyllene (18.69%), cubenol (12.53%) and ledol (11.5%) were the main constituents of the essential oil. The essential oil showed antibacterial activity against bacterial strains *Streptococcus pneumonia*, *Staphylococcus aureus*, *Streptococcus pyogenes* and *Pseudomonas aeruginosa.* Molecular docking analysis indicated that the essential oil constituents act as inhibitors of cell well synthesis and nucleic acids synthesis. It can further be explored to use in the fragrances and cosmetics.

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Conflicts of Interest

We declare that we have no conflict of interest.

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التركيب الكيميائي، في (سيلكو موليكيولار) دراسات الالتحام الجزيئي والنشاط المضاد للجراثيم في الزيوت الأساسية لزهور *Artabotrys hexapetalus*

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ملخص

عزل المكونات المتطايرة عن زهور ارتابورتيز هيكسابيتاولوس باستخدام عينة تقنية سولفنت–ترابينج والذي تم التعرف عليه من قبل تحاليل جي سي–ام اس. أكبر المكونات هي اثيل اكسيتات 53.6%، ايزوبوتيل اكسيتات (29.4) واثيل بنزوات (14.2). وقد اكتشف أن رائحة المحلول الذي تم الحصول عليه من هذه الطريقة تشبه رائحة الزهور الطازجة. بالإضافة للزيت الأساسي الناتج من أ. هيكسابيتاولوس والذي تم الحصول عليه أول مرة من الهند من قبل جهاز هيدرو ديستيلاشن يوسينج أكليفينجر تايب والذي تم تحليله من قبل جي سي–ام اس. وقد أخرجت النبتة 1.26% من الزيوت الأساسية للزهرة. وقد أسفر التحليل عن التعرف على 28 مكون تشكل 96.17% من الزيت. كما يتكون الزيت العطري في الغالب من اوكسجيناتد سيسكويتربنيس (51.91%) متبوعة ب سيسكويتربنيس (43.31%) وكميات قليلة من مونوتربينس (1.24%) ومكونات آخرى (1.34%). المكونات الرئيسية للزيت الأساسي الذي تم الحصول عليه من الزهور ل أ. هيكسابيتاولوس هي ب–كاريوفيلينى (18.69%)، كاريوفيلليني اوكسيد (14.54%)، كوبنول (12.53%) وليدول (11.5%). وقد أظهر الزيت العطري نشاطًا مضادًا للبكتريا ضد السلالات البكتيرية ستريبتوكوكوز بنومونيا، ستافيلوكوس أوريوس، ستربتوكوكوز بيوجينس أند بسويدوموناس أروجينوسا عارضة منطقة أوف انهيبيشن أوف 16.4، 15.7، 17.5 و14.5 مم وقيمة أم أي سي ب 2.5، 5.0، 2.5، 5.0 مج/مل على التوالي. وقد أشار تحليل موليكولار دوكينج أن مكونات الزيت العطري هي حمض نووي ومثبطات تخليق جدار الخلية. وعليه من المجدي إدخال ذلك في العطور ومستحضرات التجميل.

الكلمات الدالة: *Artabotrys hexapetalus*، الزيوت الأساسية، جي سي–ام اس، سيسكويتربنيس، أس كاريوفيلليني، انتيباكتيريال، الالتحام الجزيئي.

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