Asian Journal of Chemistry; Vol. 36, No. 11 (2024), 2561-2568

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2024.32570

Phytochemical Profiling and *in silico* Anticancer Activity of Plant Extract Phytocompounds against Non-Small Lung Cancer Cells

E. SUBBULAKSHMI and P. PALANISAMY*

Department of Chemistry and Research Center, Pioneer Kumaraswamy College (Affiliated to Manonmaniam Sundaranar University, Tirunelveli), Nagercoil-629003, India

*Corresponding author: E-mail: ppschem08@gmail.com

Received: 22 August 2024; *Accepted*: 12 October 2024; *Published online*: 30 October 2024; AJC-21790

In this study, the *in vitro* results confirmed the anticancer efficacy of ethanolic extracts obtained from leaves of *Ocimum basilicum*, *Aegle marmelos* and *Hibiscus rosa-sinensis*. Alkaloids, terpenoids, steroids and flavonoids were all present in significant amounts in all the ethanolic extract. The *O. basilicum* extract contained 16 phytochemicals, of which 10 showed indications of bioactivity. *A. marmelos* extract contains 20 phytocompounds, 13 of which were bioactive, whereas the *H. rosa-sinensis* extract comprised total 25 different compounds and only 11 compounds of which have bioactive properties. The study examined the phytocompounds found in the leaves of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* plants and their ability to inhibit certain lung cancer cell lines proteins (PDB ID: 6LTK). The *O. basilicum* plant leaves contain phytocompounds, which are more active against lung cancer than *A. marmelos* and *H. rosa-sinens* extracts. The molecular docking research results indicated that mesterolone (-8.8 kcal/mol) possesses significant potential as an inhibitor of the lung cancer (6LTK) cell line protein as a prospective therapeutic option and analogous to the conventional application of the studied plants.

Keywords: *Ocimum basilicum*, *Aegle marmelos*, *Hibiscus rosa-sinensis* leaf extract, GC-MS analysis, Molecular docking study.

INTRODUCTION

Cancer is one of the serious health problems worldwide. According to WHO, cancer is the second leading cause of death globally. Lung and breast cancers were the most frequently diagnosed (11.6% of all cases), while lung and colorectal cancers rank top with a high mortality rate (18.4% and 9.2% of all deaths, respectively). Consumption of tobacco was found as the primary risk factor and accounts for 22% of all cancer deaths [1]. The most common type is the former (around 80-85% of the cases) and further classified as adenocarcinoma, squamous cell carcinoma and large cell carcinoma based on the cells from which cancer had originated [2]. Various factors including difficulty in the diagnosis, tumor- and patient-specific heterogeneity of the tumor microenvironment, genomic architecture, genetic and epigenetic background and advanced metastasis pose heavy challenge in the therapeutic avenue of the NSCLC [3].

A typical phytochemical based side-effect free anticancer therapy process has to progress through the following steps: (i) evaluating the plant extracts for evaluation of the anticancer activity, (ii) purification of the active compounds based on bioassay guided fractionation, (iii) characterization of the fractions and/or compounds with *in silico*, *in vitro* and or *in vivo* potential biological activity and (iv) clinical trials of the lead for the therapeutic applications [4]. Phytochemicals can act on the cancer cells and suppress the tumor development and metastasis by various mechanisms like stabilizing the molecules that can stimulate cancer growth, boosting the immune system, reducing the inflammation, regulating hormones, inducing autophagy of the damaged cells, preventing the damage of DNA of the healthy cells, scavenging the free radicals and other means [5-7].

Medicinal plants represent a natural resource that contributes to human health and well-being. Plants and their bioactive compounds have been utilized in medicinal practices since ancient times. A variety of compounds derived from plants have been documented for their anticancer properties, with several currently being used in clinical applications [8]. From the above mentioned facts, we have investigated the phytochemical evalu-ation and *in silico* anticancer activity of ethanolic extracts

of leaves of *Ocimum basilicum, Aegle marmelos* and *Hibiscus rosa-sinensis* phytocompounds against lung (6LTK) cancer proteins cell lines.

EXPERIMENTAL

Plant materials: Fresh leaves of three medicinal plants *viz. Ocimum basilicum, Aegle marmelos* and *Hibiscus rosa-sinensis* were collected from Agastheeswaram Taluk (8º6′0″N 77º31′15″E), Kanyakumari District of India. The plant materials were taxonomically identified and authenticated by Dr. Babu, Assoc. Prof., Department of Botany, Pioneer Kumaraswamy College, Nagercoil, India. The shade dried plants were ground well using mechanical blender into fine powder and transferred into air-tight containers with proper labelling.

Extraction: Dry powdered plant leaves (50 g) were dissolved in 250 mL of ethanol using a Soxhlet extractor. Solvents were added to the Soxhlet loop during the extraction process until the solvent becomes colourless. The concentrated extracts were kept in sealed containers at room temperature until the solvent evaporated. The dried extract was kept at 4 ºC for their further experiments use in the phytochemical analysis.

Phytochemical analysis: The phytochemicals present in the ethanolic extracts leaves of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* were evaluated using a reported procedure [8]. An examination of each solvent has revealed the phytoconstituents present in the crude powder, which were extracted utilizing established methodologies.

GC-MS analysis: The phytochemistry analyses of the ethanolic extracts of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* leaves were conducted using GC-MS technique (GC-MS QP2020; Shimadzu, Japan) consisting of an auto sampler, sample injector, gas chromatograph and mass spectrometer. A capillary standard non-polar column SHRxi-5Sil-MS with the following specifications was used in the GC-MS system: 30.0 m, 0.25 mm diameter and 0.25 µm film thickness. With a 70 eV electron ionization energy, an electron ionization system was implemented. It was done using 5 µL of injection volume and 1.20 mL/min of 99.99% helium gas (split ratio: 10). The temperature of oven was set to start at 50 ºC (isothermal for 2 min) and increase to 280 ºC over a span of 10 min. At a scan interval of 0.3 s and a scan range of 50-500 *m/z*, mass spectra were recorded at 70 eV. The GC was run for 21 min in total. The percentage of each component was calculated by dividing the average peak area of each component by the total sum of all peak areas. In the NIST and WILEY libraries, the spectra of the unknown component and those of the recognized components were compared.

Molecular docking studies: The docking studies involved the interaction of proteins from lung cancer cell lines (PDB ID: 6LTK) with the chemical ingredients of a plant extract using AutoDock Vina. Initially, ChemDraw 8.0 from the Chem Office tool was used to build chemical structures of phytocompounds and assign appropriate 2D orientations. ChemBio3D was then used to reduce the energy of each chemical substances. The ligand structures were utilized as input for AutoDock Vina to perform docking simulations [9-11]. Crystal structures of the colon and cervical receptor molecules were obtained from the Protein Data Bank under the identities 6LTK. The target protein file was prepared using AutoDock 4.0's auto preparation capability (MGL tools 1.5.7), which preserved the associated protein residue. Protein preparation followed a conventional process [12], which included removing co-crystallized ligands, particular water molecules and cofactors. A grid box was built using a graphical user interface application to define the docking simulation parameters. The grid box was built with dimensions of 30, 30 and 30 grid points in the x, y and z directions, with a grid point spacing of 0.375 Å. The grid dimensions for the lung cancer protein (6LTK) were -14.813978, 34.875222 and 19.527911. The docking algorithm supplied by AutoDock Vina was used to find the best docked configuration between the ligands and proteins. During the docking process, up to nine conformers were examined for each ligand. PyMOL and Discovery Studio Visualizer were then used to analyze the interactions between the ligands and the target receptors. The conformations with the lowest free binding energy were chosen for examination, with interacting residues and hydrogen bonds shown in stick models and the ligands represented in different colours.

RESULTS AND DISCUSSION

Qualitative phytochemical analysis: The qualitative phytochemical analysis of different solvent extracts of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* leaves is shown in Table-1. In the ethanolic extract of *O. basilicum*, saponin and reducing sugars were found at higher concentrations. It was found that

TABLE-1
PRELIMINARY PHYTOCHEMICAL SCREENING OF ETHANOLIC EXTRACT OF POWDERED LEAVES OF THREE PLANTS

S. No.	Phytochemicals	*Ocimum basilicum*	*Aegle marmelos*	*Hibiscus rosa-sinensis*
1	Terpenoids (Chloroform test)	++	+	+++
2	Carbohydrates (Molisch's test)	–	+	–
3	Phenolic compounds (Ferric Chloride test)	++	+++	++
4	Steroids (Chloroform test)	++	+	++
5	Saponin (Foam test)	+++	++	+
6	Alkaloids (Wagner's test)	++	+++	++
7	Flavonoids (Alkaline reagent test)	+	–	++
8	Tannins	–	+	+
9	Reducing sugar (Fehling's test)	+++	+++	–
10	Proteins (Millon's test)	–	++	–

Note: + = present in small concentration; ++ = present in moderately high concentration; +++ = present in very high concentration; – = absent

terpenoids, phenolic compounds, steroids and alkaloids were present in moderate concentrations, whereas the flavonoids is present in lower concentrations. Proteins, carbohydrates and tannins were not present in these extracts. Alkaloids, phenolic compounds and reducing sugars were present in higher concentrations in the ethanolic extract of *A. marmelos* leaves, whereas proteins and saponnin were present in moderate levels. The terpenoids, steroids, carbohydrates and tannins were replaced in smaller quantities. The ethanolic extract of *H. rosa-sinensis* leaves revealed higher quantities of terpenoids but proteins, steroids, alkaloids and flavonoids were present in moderate levels. The tannins and saponins have been displaced in lower quantities. The extract exhibited no carbohydrates, reducing sugars and proteins.

Identification of phytocompounds: The ethanolic extracts of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* leaves were subjected to the GC-MS analysis, which identified the presence of phytochemicals compounds (Fig. 1). Table-2 displays the chemical compounds together with their molecular weight, molecular formula, retention time and concentration (peak area percentage). The spectra of the unknown components were compared with those of known components using the NIST and WILEY libraries.

Among the bioactive substances included in *O. basilicum* extracts are 1,3-dichloropropane, caryophyllene, farnesol, 2,6-di-*tert*-butyl-4-methylphenol, 3-eicosyne, capsidiol, *n*-octyl-1*H*-imidazole-1-carboxamide, mesterolone, palmitic acid and brexanolone. In *A. marmelos* extract, only 14 out of isolated 20 phytocompounds were found to be bioactive compounds. These were 1-chloropropane, 4-vinylphenol, benzyl acetate, eugenol, toliprolol, apiole, zingerone, myristic acid, neophytadiene, erucic acid, phytol, palmitic acid and dihomo-γ-linolenic

TABLE-2
GC-MS ANALYSIS OF PHYTOCOMPOUNDS FROM ETHANOLIC EXTRACT OF *Ocimum basilicum*, *Aegle marmelos* AND *Hibiscus rosa-sinensis* LEAVES

Retention time (min)	Peak area (%)	m.f.	m.w.	Name of the compound	Secondary metabolism
			Ocimum basilicum		
4.350	15.54	$C_3H_6Cl_2$	112	1,3-Dichloropropane	Alkane
14.789	1.06	$C_{15}H_{24}$	204	Caryophyllene	Sesquiterpenes
17.416	3.32	$C_{15}H_{26}O$	222	Farnesol	Sesquiterpenes
17.589	4.27	$C_{15}H_{24}O$	220	2,6-Di-*tert*-butyl-4-methylphenol	Phenols
18.955	29.16	$C_{12}H_{21}N_3O$	223	N-Octyl-1*H*-imidazole-1-carboxamide	Imidazole
20.440	2.91	$C_{20}H_{38}$	278	3-Eicosyne	Fatty acids
21.292	3.11	$C_{15}H_{24}O_2$	236	Capsidiol	Sesquiterpenoid
21.509	2.60	$C_{20}H_{32}O_2$	304	Mesterolone	Steroids
21.908	1.03	$C_{16}H_{32}O_2$	256	Palmitic acid	Fatty acids
22.350	0.58	$C_{21}H_{34}O_2$	318	Brexanolone	Steroids
34.521	2.31	$C_{30}H_{48}O_3$	456	Ursolic acid	Triterpenoids
			Aegle marmelos		
4.360	44.57	C_3H_7Cl	78	1-Chloropropane	Alkane
12.225	0.75	C_8H_8O	120	4-Vinylphenol	Phenolic compounds
13.610	0.37	$C_9H_{10}O_2$	150	Benzyl acetate	Ester
15.645	1.20	$C_{10}H_{12}O_2$	164	Eugenol	Phenolic compounds
17.155	1.21	$C_{13}H_{21}NO_2$	180	Toliprolol	Aromatic ether
17.495	5.86	$C_{12}H_{14}O_4$	222	Apiole	Amino alcohol
18.885	054	$C_{11}H_{14}O_3$	194	Zingerone	Phenolic derivatives
19.640	1.95	$C_{14}H_{28}O_2$	228	Myristic acid	Carboxylic acid
20.420	4.39	$C_{20}H_{38}$	278	Neophytadiene	Terpenes
20.685	0.60	$C_{22}H_{42}O_2$	338	Erucic acid	Carboxylic acid
20.895	1.11	$C_{20}H_{40}O$	396	Phytol	Terpenes
21.955	11.57	$C_{16}H_{32}O_2$	256	Palmitic acid	Carboxylic acid
23.825	23.20	$C_{20}H_{34}O_2$	306	Dihomo-γ-linolenic acid	Carboxylic acid
34.651	2.16	$C_{13}H_{12}O_4$	232	1-Hydroxy-5,7-dimethoxy-2-naphthalene-carboxaldehyde	Ester
			Hibiscus rosa-sinensis		
13.237	1.74	$C_{10}H_{14}O$	150	Carvacrol	Terpenes
14.154	2.12	$C_{10}H_{12}O_2$	164	Eugenol	Caffeic acids
17.145	1.20	$C_{10}H_{12}O_3$	180	Propylparaben	Parabens
17.657	0.68	$C_{12}H_{16}O_3$	208	α-Asarone	Anisoles
18.875	1.73	$C_{11}H_{14}O_3$	194	Zingerone	Catechols
19.491	1.58	$C_{11}H_{16}O_3$	196	2,6-Dimethoxy-4-propylphenol	Phenols
19.615	0.78	$C_{14}H_{28}O_2$	228	Myristic acid	Fatty acid
20.424	0.76	$C_{38}H_{74}O_2$	563	Icosyl oleate	Ester
20.685	5.28	$C_{20}H_{38}$	278	3-Eicosyne	Fatty acids
20.894	9.69	$C_{20}H_{40}O$	296	Phytol	Terpenes
21.933	22.65	$C_{16}H_{32}O_2$	256	Palmitic acid	Fatty acids
33.534	2.41	$C_{15}H_{10}O_8$	318	Gossypetin	Flavanone

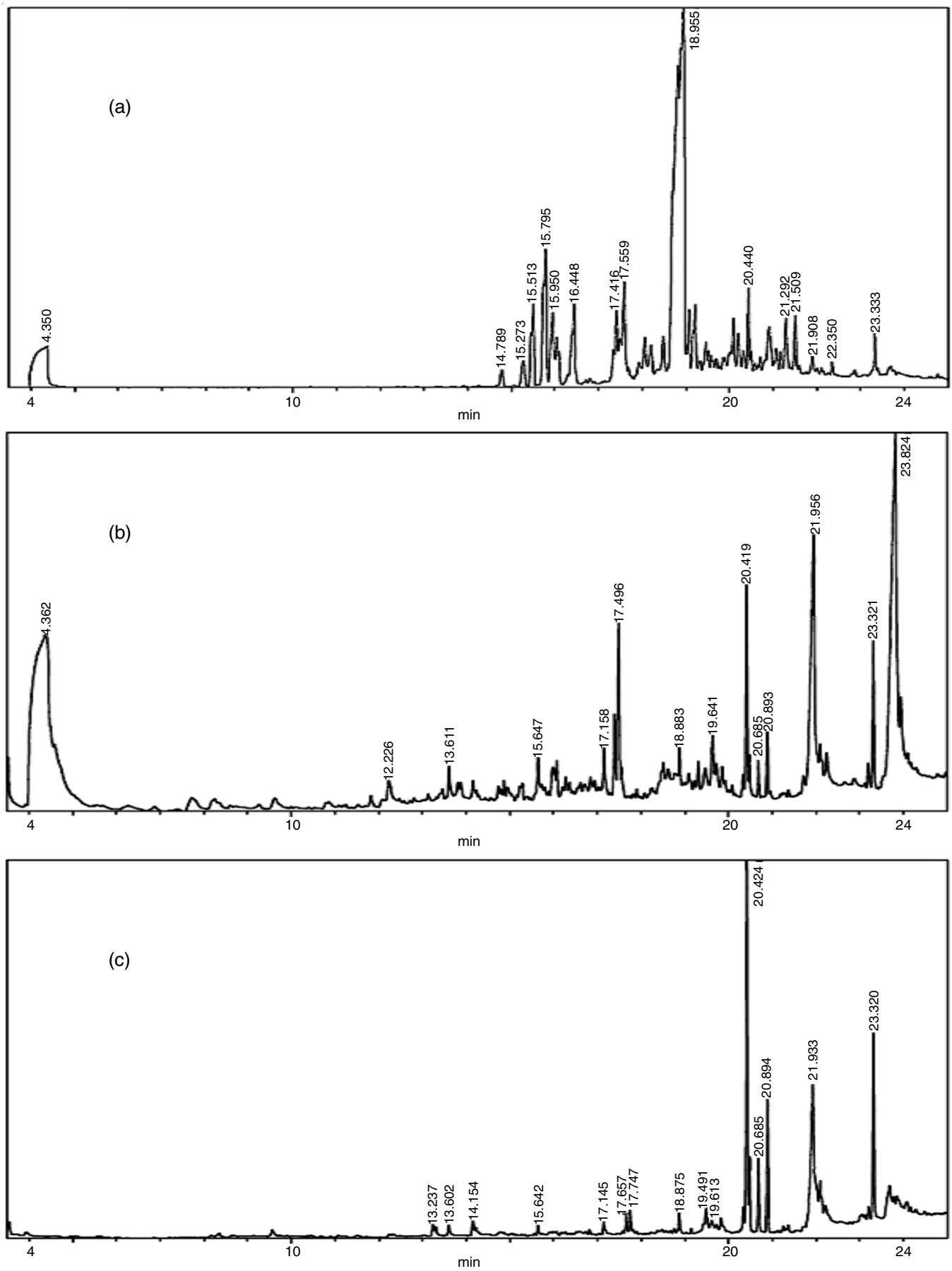

Fig. 1. GC-MS chromatogram of (a) *Ocimum basilicum*, (b) *Aegle marmelos* and (c) *Hibiscus rosa-sinensis* leaves ethanol extracts

acid. In *H. rosa-sinensis* extracts, only 12 out of 25 compounds were bioactive. The main bioactive phytocompounds include carvacrol, eugenol, propylparaben, α-asarone, 2,6-dimethoxy-4-propylphenol, zingerone, myristic acid, icosyl oleate, 3-eicosyne, phytol and palmitic acid (Table-2).

Molecular docking studies: The computational methods use molecular docking to provide predictive insights into the interactions between small compounds and receptors. The *in silico* antibacterial activity was analyzed using AutoDock Vina software. The lung cancer activity of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* leaves extract phytocompounds against the selected lung cancer cell lane proteins (PDB ID: 6LTK) was studied. Gemcitabine as was used reference lung cancer drugs.

Among the isolated biologically active phytocompounds from *O. basilicum* ethanolic extracts, only 10 phytocompounds demonstrated anticancer efficacy, which are comparable to that of the reference drugs. Table-3 listed the docking scores and binding interactions for standard compounds and ligands found in phytocompounds from *O. basilicum* leaves. Docking scores of non-small lung cancer protein cell lines (6LTK) indicate that some ligands have shown activity similar to standards. The binding affinities of the ligands that target protein cell lines associated with lung cancer range from -4.8 to -8.8 kcal/mol. The binding affinities of standard gemcitabine for lung cancer cell types were -7.1 kcal/mol. Among these drugs, three phytocompounds have low anticancer activity [farnesol, 3-eicosyne and palmitic acid], three phytocompounds have moderate activity [caryophyllene, 2,6-di-*tert*-butyl-4-methylphenol, N-octyl-1*H*-imidazole-1-carboxamide] and four phytocompounds have highest anticancer activity [capsidiol, mesterolone, ursolic acid and brexanolone]. Furthermore, the results of the molecular docking analysis showed the high potential of mesterolone (-8.8 kcal/mol) as a lung cancer (6LTK) cell line protein inhibitor (Fig. 2).

The anticancer activity of 13 phytocompounds isolated from the ethanolic extract of *A. marmelos* leaves was found to be similar to that of the reference drugs. Several ligands have shown activity comparable to standards based on docking score investigations of non-small lung cancer protein cell lines (6LTK). The ligands that target protein cell lines linked to lung cancer have binding affinities ranging from -4.8 to -6.2 kcal/mol (Table-4). Among these drugs, nine phytocompounds have low anticancer activity [4-vinylphenol, benzyl acetate, apiole, myristic acid, neophytadiene, erucic acid, phytol, palmitic acid and dihomo-γ-linolenic acid] and four phytocompounds have moderate activity [eugenol, toliprolol, zingerone and 1-hydroxy-5,7-dimethoxy-2-naphthalene-carboxaldehyde].

Twelve phytocompounds present in the ethanolic extracts of *H. rosa-sinensis* leaves were found to be physiologically active. Surprisingly all twelve phytocompounds exhibited anticancer efficacy comparable to that of the reference drug. The ligands with binding affinities ranging from -4.8 to -8.7 kcal/mol are directed towards protein cell lines associated with lung cancer (Table-5). For lung cancer cell types, standard gemcitabine exhibited significant binding affinities of -7.1 kcal/mol. Among these drugs, six phytocompounds have low anticancer activity [carvacrol, α-asarone, myristic acid, 3-eicosyne, phytol, palmitic acid], five phytocompounds have moderate activity [eugenol, propylparaben, zingerone, 2,6-dimethoxy-4-propylphenol, icosyl oleate] and one phytocompounds has high activity (gossypetin). The molecular docking analysis data also showed

TABLE-3
MOLECULAR DOCKING ANALYSIS OF *Ocimum basilicum* LEAVES PHYTOCOMPOUNDS AGAINST LUNG CANCER CELL LINE PROTEIN (6LTK)

Phytocompound	Binding energy	Binding interactions		
		Hydrogen bond	Hydrophobic bond	Electrostatic bond
Caryophyllene	-6.6	ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, ALA218	ARG217, ALA218, ILE207, TYR194, PHE200	ARG217, TYR194
Farnesol	-5.4	ALA214, ASP211, ARG217, PRO213, ARG217, SER186, SER188, ALA218, GLN220, ASP221, ALA218, ARG154, PRO199, ARG154, PRO202	ALA214, ILE207, PRO208, ARG217, ALA218, PRO199, PRO202, TYR194, ARG217, PHE200	ARG217, TYR194
2,6-Di-*tert*-butyl-4-methylphenol	-6.2	ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, ALA218	ARG217, TYR194, PHE200 - ARG217, ALA218, ILE207	ARG217, TYR194
N-Octyl-1*H*-imidazole-1-carboxamide	-6.7	PHE172, ASP205, ASP205, ILE170, ARG217, PRO213, ILE185, SER188, GLN220, ILE206, ASP205	ALA214, PRO208, ILE206, TYR194, PHE200	ARG217, TYR194
3-Eicosyne	-4.8	ALA174, ILE207, ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, GLN233, ILE207, PHE172, ASP211, PRO213, SER188, ALA218, GLN220, ASP221	ALA174, PRO208, ALA218-B: ALA214, ARG217, ILE206, ILE207, ARG217	ARG217, TYR194
Capsidiol	-7.2	ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, ALA218, ILE206	ARG217, ALA218, ILE207, TYR194, PHE200	ARG217, TYR194
Mesterolone	-8.8	ARG154, CYS150, PHE197, PRO199, PRO202, TYR158, ILE206, PRO202, PHE197	PRO199, PRO202, TYR158, ARG154	
Palmitic acid	-4.8	GLY203, PHE204, PHE204	ARG217, ALA218, PHE200	–
Ursolic acid	-8.5	PHE204	PHE172, PHE204, ILE170, MET201	–
Brexanolone	-8.4	PHE172, ASP205, ILE170, ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, ASN223, ASP221, VAL224, ASP221, ASP205	ALA218, ILE207, TYR194, ARG217, PHE200, ARG217	ARG217, TYR194

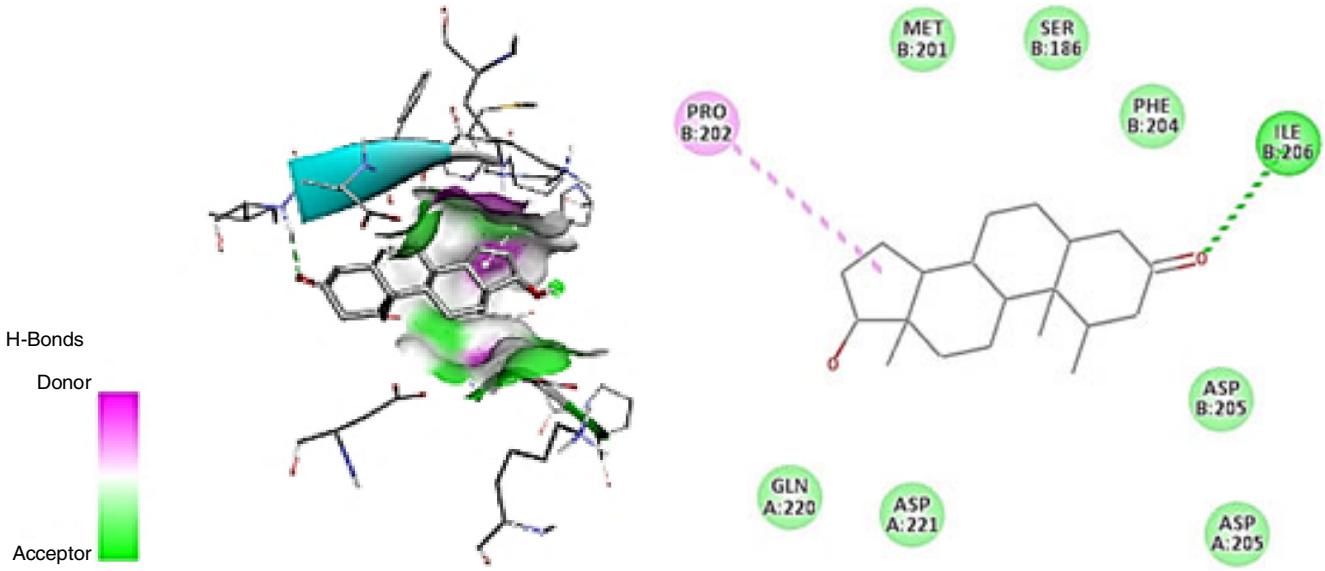

Fig. 2. 3D, 2D and finding interaction of mesterolone

TABLE-4
MOLECULAR DOCKING ANALYSIS OF *Aegle marmelos* LEAVES PHYTOCOMPOUNDS AGAINST LUNG CANCER CELL LINE PROTEIN (6LTK)

Compound	Binding energy	Binding interactions		
		Hydrogen bond	Hydrophobic bond	Electrostatic bond
4-Vinylphenol	-5.3	PHE177, GLU230, VAL229, ILE265, ASP263, TYR85, SER295, LYS292, GLY296, TYR323, LYS292, THR322	PHE177, ALA87, LYS292, LYS292, ILE265, LE265, PHE177, ILE265	ARG413, GLU235, GLU235, PHE177
Benzyl acetate	-5.8	GLY142, THR322, TYR323	PHE177, ILE265	
Eugenol	-6.0	ARG217, PRO213, SER186, SER188, GLN220, LE206, ILE206	ILE206, ARG217, TYR194, PHE200	ARG217, TYR194
Toliprolol	-6.2	ALA174, ILE207, ILE207, PHE172, ARG154, PRO202, MET201	ILE206, VAL171, ILE207, ALA214, PRO208, ALA218, ILE207, PRO202, PRO199, PRO208, ILE206, PHE204, MET201	–
Apiole	-5.9	ILE206, ARG217, ASP205, ALA214	ALA214, ALA218, ILE207, ARG217, ILE206, PRO208, ILE206	–
Zingerone	-6.0	ARG180, ARG180, THR322, PRO406	TYR85, LYS405	GLU235
Myristic acid	-5.7	ARG180, GLY320, SER321	VAL143, LYS292, ILE265, PHE177	–
Neophytadiene	-5.2	ARG217, SER186, SER188, ALA218, ALA214, GLN220, ASP221, ALA218	ARG217, ALA218, ILE207, ILE206, TYR194, ARG217, B: PHE200	ARG217, TYR194
Erucic acid	-5.3	ARG180, LYS292, THR322	TYR85	–
Phytol	-5.5	MET201, SER186	ARG217, ALA218, ILE207, PRO208, ILE206	–
1-Hydroxy-5,7-dimethoxy-2-naphthalene-carboxaldehyde	-6.5	ARG217, ALA214, ALA218, ASP205	ARG217, ALA218, ILE206	–
Palmitic acid	-4.8	GLY203, PHE204, PHE204	ARG217, ALA218, PHE200	–
Dihomo-γ-linolenic acid	-5.7	ARG217, SER186, SER188, ALA218, ALA214, GLN220, ARG217, ASP221, ALA218, PHE204, MET201	PHE172, PHE204, ARG217, ALA218, ILE207, ILE206, TYR194, PHE200, PHE204, ILE170, MET201	ARG217, TYR194

that gossypetin (-8.7 kcal/mol) has a great potential as a lung cancer (6LTK) cell line protein inhibitor (Fig. 3).

Conclusion

The ethanolic extracts obtained from *Ocimum basilicum*, *Aegle marmelos* and *Hibiscus rosa-sinensis* leaves contain several bioactive compounds, which have significant anticancer efficacy. The highest concentrations of terpenoids, alkaloids, flavonoids, saponin, fatty acids, phenolic compounds and steroids were detected in the ethanolic extracts of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* leaves based on qualitative analysis. The *Ocimum basilicum* extracts contained sixteen phytochemicals, of which ten showed indications of bioactivity. *A. marmelos* extracts included twenty phytocompounds, thirteen of which

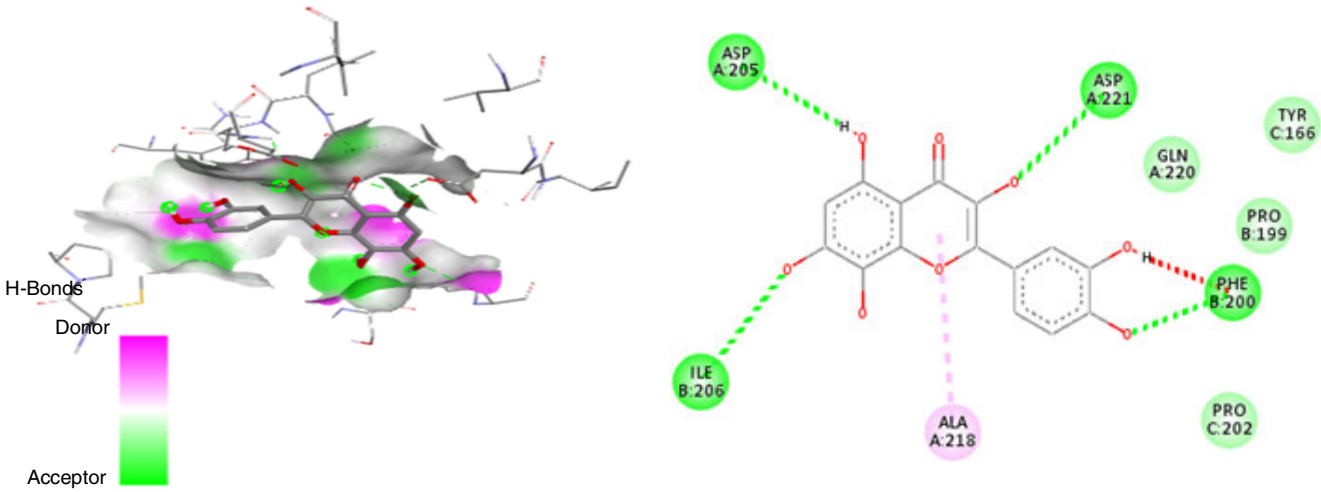

Fig. 3. 3D, 2D and finding interaction of gossypetin

TABLE-5
MOLECULAR DOCKING ANALYSIS OF *Hibiscus rosa-sinensis* LEAVES PHYTOCOMPOUNDS AGAINST LUNG CANCER CELL LINE PROTEIN (6LTK)

Compound	Binding energy	Binding interactions		
		Hydrogen bond	Hydrophobic bond	Electrostatic bond
Carvacrol	-5.7	ARG217, ALA214	ILE207, ARG217, ALA218	–
Eugenol	-6.0	ARG217, PRO213, SER186, SER188, GLN220, LE206, ILE206	ILE206, ARG217, TYR194, PHE200	ARG217, TYR194
Propylparaben	-6.6	ARG180, PHE177	ILE265, PHE177, LYS292, TYR323	–
α-Asarone	-5.7	TYR85, ARG180, LYS405	LYS405, TYR85, PHE177	GLU235
Zingerone	-6.7	ARG154, PHE204, ARG217, PRO213, ARG217, ILE185, SER188, GLN220, MET201	TYR194, ARG217, PHE200, PHE204, ILE170, MET201, PHE172, PHE204	ARG217, TYR194
2,6-Dimethoxy-4-propylphenol	-6.7	ARG180, LYS292, GLU144	VAL143, ILE265, PHE177, TYR323	–
Gossypetin	-8.7	ASP221, PHE200, ILE206, ASP205	ALA218	–
Myristic acid	-5.7	ARG180, GLY320, SER321	VAL143, LYS292, ILE265, PHE177	–
Icosyl oleate	-6.3	ARG217	ALA174, ILE206, PRO208, ARG217, ALA174, ARG217, ALA218, ILE206, ILE207	–
3-Eicosyne	-4.8	ALA174, ILE207, ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, GLN233, ILE207, PHE172, ASP211, PRO213, SER188, ALA218, GLN220, ASP221	ALA174, PRO208, ALA218; B: ALA214, ARG217, ILE206, ILE207, ARG217	ARG217, TYR194
Phytol	-5.5	MET201, SER186	ARG217, ALA218, ILE207, PRO208, ILE206	–
Palmitic acid	-4.8	GLY203, PHE204, PHE204	ARG217, ALA218, PHE200	–
Gemcitabine (Standard drug)	-7.1	PHE172, ASP205, ILE170, ARG217, PRO213, SER186, SER188, ALA218, ALA214, GLN220, ASP221, SER186, LEU182, ALA218, MET201	ALA218, ILE207, TYR194, ARG217, PHE200, PHE204, MET201	ARG217, TYR194

were bioactive. Twenty-five chemicals total, eleven of which were bioactive, were found in the extracts of *H. rosa-sinensis*. The study also examined the phytocompounds found in the leaves of *O. basilicum*, *A. marmelos* and *H. rosa-sinensis* plants and their ability to inhibit certain lung cancer cell lane proteins (PDB.ID: 6LTK). Four phytocompounds in *O. basilicum* have the highest level of anticancer action, three have moderate activity and three have low activity. Four phytocompounds in *A. marmelos* show moderate anticancer activity, whereas nine have low activity. Six phytocompounds of *H. rosa-sinensis* have modest anticancer activity, five have moderate activity and one has significant activity. According to comparison studies, *O. basilicum* plant leaves contain phytocompounds that are more active against lung cancer than *A. marmelos* and *H. rosa-sinensis*. Though these results are positive, however, more study is needed especially to separate and identify the active major component of the product and evaluate its cost-benefit ratio as well as its capacity to cure lung cancer cells.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

REFERENCES

1. D.N. Sinha, R.A. Suliankatchi, P.C. Gupta, T. Thamarangsi, N. Agarwal, M. Parascandola and R. Mehrotra, *Tob. Control*, **27**, 35 (2018); https://doi.org/10.1136/tobaccocontrol-2016-053302
2. A. Teramoto, T. Tsukamoto, Y. Kiriyama and H. Fujita, *BioMed. Res. Int.*, **2017**, 4067832 (2017); https://doi.org/10.1155/2017/4067832
3. A.M. Cryer and A.J. Thorley, *Pharmacol. Ther.*, **198**, 189 (2019); https://doi.org/10.1016/j.pharmthera.2019.02.010
4. M.A.T. Phan, J. Paterson, M. Bucknall and J. Arcot, *Crit. Rev. Food Sci. Nutr.*, **58**, 1310 (2018); https://doi.org/10.1080/10408398.2016.1254595
5. W.L. Lee, J.Y. Huang and L.F. Shyur, *Oxid. Med. Cell. Longev.*, **2013**, 925804 (2013); https://doi.org/10.1155/2013/925804
6. X.B. Yan, T. Xie, S.D. Wang, Z. Wang, H.Y. Li and Z.M. Ye, *Int. J. Clin. Exp. Med.*, **11**, 1615 (2018).
7. L. Cao, X. Wang, G. Zhu, S. Li, H. Wang, J. Wu, T. Lu and J. Li, *Integr. Cancer Ther.*, **20**, 15347354211061720 (2021); https://doi.org/10.1177/15347354211061720
8. R.N.S. Yadav and M. Agarwala, *J. Phytol.*, **3**, 10 (2011).
9. X. Yang, P. Neta and S.E. Stein, *Anal. Chem.*, **86**, 6393 (2014); https://doi.org/10.1021/ac500711m
10. H.J. Hubschmann, Handbook of GC-MS: Fundamentals and Applications, John Wiley & Sons (2015).
11. S. El-Hddad, M. Sobhy, A. Ayoub and K. El-Adl, *J. Biomol. Struct. Dyn.*, **41**, 9267 (2023); https://doi.org/10.1080/07391102.2022.2148000
12. L. Martin, M.P. White, A. Hunt, M. Richardson, S. Pahl and J. Burt, *J. Environ. Psychol.*, **68**, 101389 (2020); https://doi.org/10.1016/j.jenvp.2020.101389