JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

"STUDY OF COMPUTER-BASED MOLECULAR DOCKING OF CURRY LEAVES IN DRUG DESIGN AND DEVELOPMENT"

Miss. Shambala Satappa Gilbile[1], Miss. Akanksha Tanaji Chopade[1*],Miss. Snehal Prakash Dhabale[1]. Miss. Chetana V. Bugadikattikar[2].

1Student 2Assistant professor

Yashwant Redekar College of Pharmacy (B. Pharm & D. Pharm), Nesari, Kolhapur Maharashtra 416504

ABSTRACT

The Rutaceae family member Murrayakoenigii (MK) has numerous health advantages. From various portions of this plant, over 88 carbazole alkaloids, terpenoids, and other nutrients have been discovered so far. This study summarises existing knowledge on the function of MK and its components in the prevention and treatment of cancer. In a number of malignant cell lines (colon, lung, liver, skin, prostate, breast, etc.), certain animal models, and a number of aberrant pathways related to apoptosis, growth (JAK-STAT, mTOR), and cell cycle, MK and its constituents have been shown to target. As a result, the current study emphasises additional views as well as the anticancer mechanism of MK and its phytoconstituents. The anti-cancer properties of MK and its phytoconstituents justify its multi-institutional clinical use.The anti-cancer properties of MK and its phytoconstituents call for multi-institution clinical trials to be conducted as soon as possible. The potential for significantly less expensive cancer treatments Then be better, especially for cancer patients who are socioeconomically weaker, The globe.

KEYWORDS: Murraya Koenigii, Bacteria, Inhibition zone, Antimicrobial effects.

INTRODUCTION

Moenigii Murraya Spreng, also known as "Surabhinimba" in Sanskrit, is a member of the Rutaceae family. Curry leaves go by various names depending on who you ask. Ethnic, Bengalis are referred to as "Barsunga" in Bengali, while Karivempu is known in Tamil and As Kurrypatte.The genus Murraya contains fourteen species worldwide. It is only possible to find Murraya koenigii Spreng and Murrayapaniculata (Linn) in India.Murraya koenigii, a member of the Rutaceae family, is more Greater than 1600 species and 150 genera. This plant's leaves have been frequently utilised in Indian cuisine and the chemical that gives it its fragrant flavour P- gurjunene, P-caryophylene, P- elemene, and O- phellandrene2 are characteristics. Pinene, caryophyllene, phellandrene, and caryophyllene have all been found to have Ability to prevent food from spoiling either individually or in combination . The writer claims that each of Murraya koenigii's three morphotypes offers a unique threat. the flavor's potency. The Murrayakoenigii regular type grows the most quickly. a plant having attractive leaves that are a dark green tint. A dwarf variety development like a shrub, its branches extend out and appear bushy, and its leaves are illuminated It is a light shade of green, slightly higher than standard kind, and emits its unique scent. It The brown kind has the thickest and thinnest leaf structure and is the most aromatic. a dark brown hue.

Introduction of cancer

Definition

A set of disorders known as cancer involve abnormal cell proliferation and have the potential to invade or spread to other bodily parts. The sickness that develops as a result of cellular alterations is known as cancer. Induces unchecked cell growth and division.

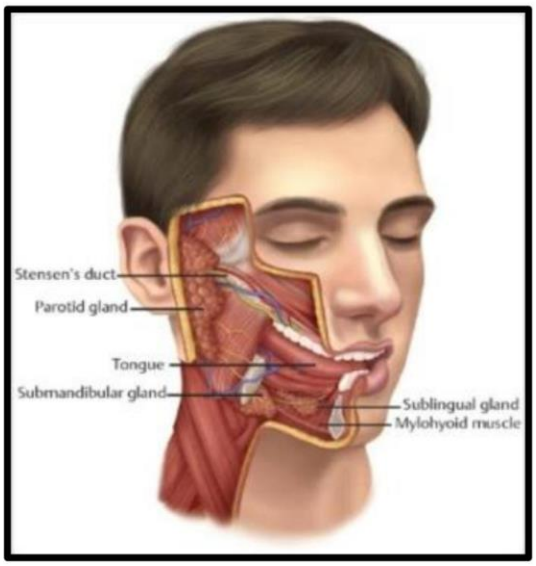
Cancer type:

The most common cancer kind Are cancers like melanoma, lymphoma, lymphosarcoma, and leukaemia There are two methods to categorise cancer. Histological type: Tissue types from which cancer develops By primary site: The area of the body where cancer first manifested itself

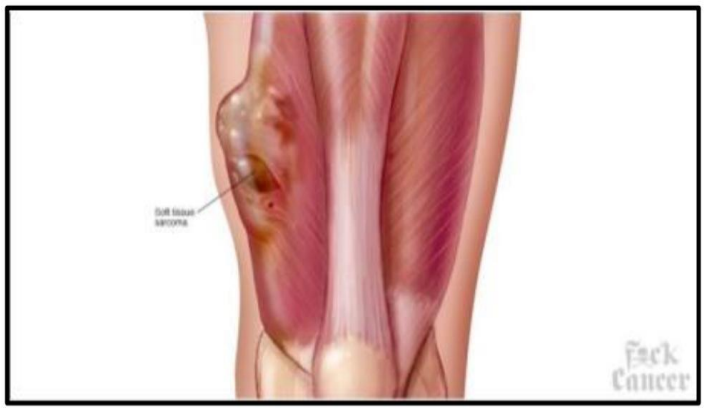
1. Histological category Cancer comes in 100 various varieties. These are categorised into six broad categories.

Carcinoma: This term describes cancer that starts in epithelial tissue. Epithelial tissue is present in the skin, the covering and linning of organs, and other parts of the body. infernal pathways like the digestive system Two major subtypes of carcinoma exist; Adenocarcinoma: They grow in an organ or gland. They happen. mucous membranes.

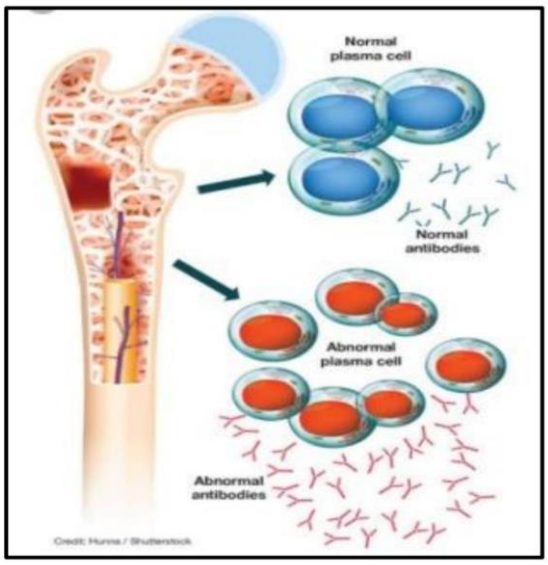
Mucosa: Squamous cell cancer in the mucosa It comes from the squamous epithelium. Occurs throughout much of the body.



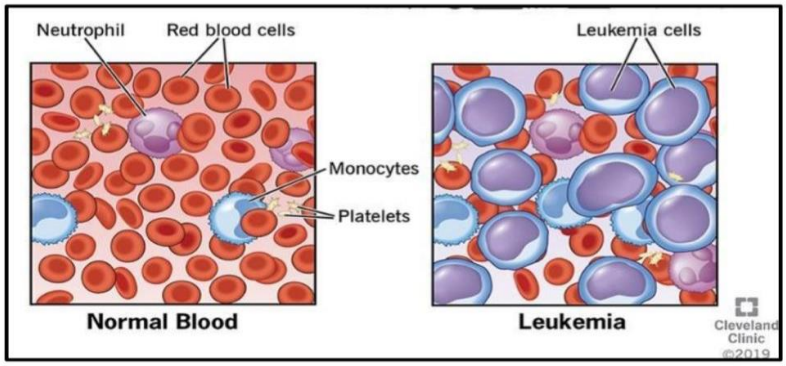
SARCOMA: Sarcoma is the name for cancer that develops from connective and supporting tissue. The tissue, including muscles, fat, tendons, cartilage, bones, and more. Sarcoma growths Typically look like the tissue in which they are found.



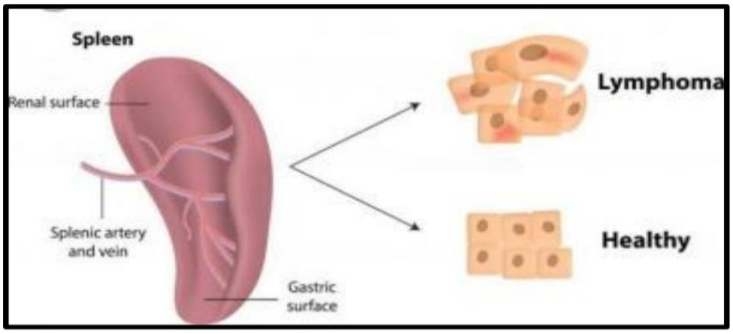
MYELOMA: Myeloma is a malignancy that develops in bone marrow cells.



LEUKEMIA: Leukemia is a type of cancer that affects the blood or the fluids. This is bone marrow cancer. The condition frequently linked to excessive production of immature Undeveloped white blood cells.



LYMPHOMA: Lymphoma is referred to as a solid cancer at times. It grows in lymphatic system glands or nodes. We call these extranodal lymphomas. Additionally, it could happen in the brain, breast, or stomach.



OBJECTIVE:

Study's goal is to examine the extract's extraction procedure. to research extraction's phytochemical screening. to investigate the anti-cancer properties of plant curry leaf extract.

Introduction of plant

The curry tree, Murrayakoenigii or Berger koenigii, is a tropical to sub-Tropical tree in the family Rutaceae (the rue family, which includes rue, citrus, And satinwood), The plant is also sometimes called sweet neem, though M. Koenigii is in a different family to neem, Azadirachta indica, which is in the related Family Meliaceae, Kingdom: Plantae, Clade: Tracheophytes, Clade: Angiosperms, Clade: Eudicots, Clade: Rosids, Order: Sapindales, Family: Rutaceae, Genus: Murraya, Species: M. koenigii Binomial name: Murrayakoenigii, Synonym: Bergerakoenigii L., Camuniumkoenigii (L.) Kuntze

Cultivation and collection

The primary curry leaf fruit season is from July through August. The seeds should be pulped and sowed in nursery beds or plastic bags three to four days after the fruits are collected. Seedlings that are one year old are acceptable for planting. There is one seedling sown.within the pit's centre.

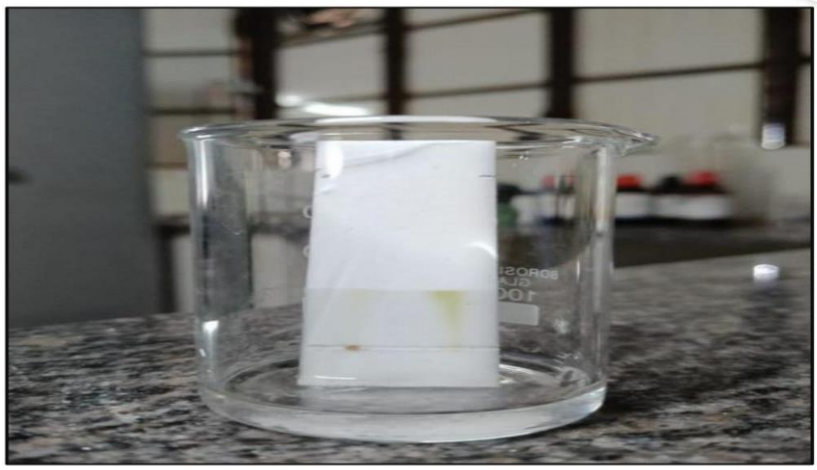
Description

Curry leaf, also known as Murrayakoenigii, is a small, tropical to sub-tropical tree or shrub that normally grows to be 6 to 15 feet tall. It is famous for its spicy, aromatic curry leaves, which are a key ingredient in Indian and Asian cuisine. Many vegetable dishes include curry leaves. Curry leaf, commonly the Rutaceae family Evergreen, fragrant leaf Height range: 6 to 15 feet

Chemical constituents

The oils from the curry leaves were found to contain mostly oxygenated monoterpenes. Using GC and GC-MS 33 constituents were found with linalool (32.83%), elemol (7.44%), geranyl acetate (6.18%), myrcene (6.12%), allo-ocimene (5.02), α-terpinene (4.9%), and (E)-β-ocimene (3.68%) as the main compounds.

Thin layer chromatography (TLC)



Thin Layer Chromatography is a technique used to isolate non-volatile mixtures.The experiment is conducted on a sheet of aluminium foil, plastic, or glass which is coated with a thin layer of adsorbent material. The material usually used is aluminium oxide, cellulose, or silica gel.On completion of the separation, each component appears as spots separated vertically. Each spot has aretention factor (RF) expressed as:

RF value: RF = dist. Travelled by sample/dist. Travelled by solvent

The factors affecting retardation factor are the solvent system, amount of material spotted, absorbent and temperature. TLC is one of the fastest, least expensive, simplest and easiest chromatography techniques.

Material and Methods:

2.1. Plant Material. Fresh leaves of curry leaf were collected locally from three different province. The leaves were shade-dried and were powdered using mechanical grinder. These powered materials were used for further analysis.

2.2. Preparation of Extract. Leaf samples (0.25 g) were extracted with 20 mL of methanol on a shaker for 2 h at room temperature. The extract solution was treated with 5 mL of hydrochloric acid (6 M) and refluxed for 2 h at 90 0 C. The hydrolysed samples were cooled to room temperature and filtered through a 0.45 gm membrane

1) Extraction Methods

Plant Material:Fresh leaves of Murrayakoenigi were collected arroundkuantan, Pahang ana only fresh leaves with the finest quality were used as a law material in this research work Essential oil Extraction

2) Pre - treatment methods: The collected fresh leaves of Murrayakoenigii were washed to remove the dirt on the surface of the Leaves It is to make sure that no any other impurities stick to the Hungry Koeniggiileaves.The excess water moisture on the leaves surfaces werethen adsorbed using paper towelThe extraction was carried out using only fresh Leaves

3) Steam Distillation (SD): 200g of fresh leaves of MurrayaKoenigii were steamed in the upper round flask With 1000 ml of distilled water until oil was distillate the operating temp. Was 130.4Each extraction was performed within the period of extraction time of3, 4, 5, 6, 7 18 4 9 bxThe essential oil was then separatedfrom the hydrosol by using Diethyl! Ether as a solvent (verma, 2012)

4) Maceration:The essential oil was extracted using steam distillation and hydro-distillation. The Amount of leaves and water used were 200 gram and 2 ml. The time of extraction For both methods were between 3 to 9 hours.This is an extraction procedure in Which coarsely powdered drug material, either leaves or stem bark or Root bark, is Placed inside a container; the menstruum is poured on top until completely covered The Drug material. The container is then closed and kept for at least three days.

5) Analysis of essential oil IJ Gas chromatography – Mass spectrometry (GC – MS) :for the determination of The chemical constituents contained in the essential oil of Murraya Koenigii leaves- Gas chromatography – Mass spectrometry.

6) Repellency Test: The repellence of the volatile oil was evaluated using the instrument that has been Modified from Y – tube olfactometer. This instrument was made from a transparent Prospex + has been fabricated with a shape of Y.The lest has been done by using Blattana (sin number) .The observation during the test way recorded The percentage of repellency

was calculated based on theformula : 1. Repellence = [CC-I) / Cx 100] where C is the total of Blattuna that landed on the control+ I is the number of Blattoria that landed on the treated area of the essential oil (Nkomo , 2012

Methodology:

1) Preparation of crude extract:

Fresh Piper curry leaves were washed properly in distilled water, air dried for 10 days at room temperature and powdered. Then, the dried leaf powder was extracted by three different extraction methods, namely Soxhlet extraction, sonication and maceration using acetone as solvent.All the extractions were carried out from 100 g of the powdered leaf sample in 500 mL of acetone (99.7%, v/v). Soxhlet extraction was conducted using acetone as solvent (56 °C) for 8 h; maceration was carried out at the room temperature for 72 h with occasional stirring. Sonication was carried out at room temperature for 1 h using Sonics Vibra cell sonicator with a power level at 135 W and sonication Frequency at 40 kHz. All the extracts obtained from different methods were stored in an air tight Containerat 4 °C for analysis.

2) Preparation of methanol extract:

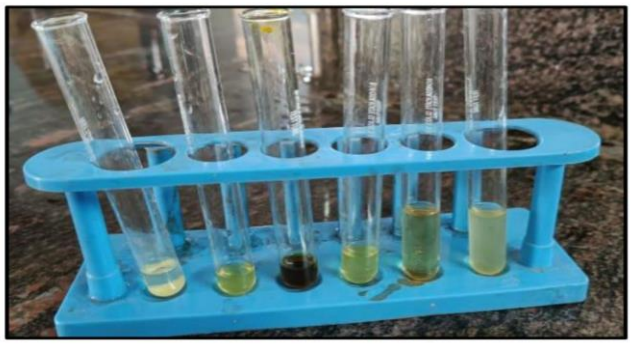
Freshly cut curry leaves were lyophilized to remove any moisture present. Freeze-dried leaves were soaked in methanol overnight for three consecutive days. The supernatant was collected daily, concentrated under reduced pressure and lyophilized to remove any traces of moisture. The dried CLE was then stored at 80°C. Batch-to-batch variation was assessed by quantitating HC content via)-ultraviolet (UV) analysis, and no significant variations were observed in the three batches process.

3) Preparation of water extract: Powdered leaves were stirred using magnetic stirrer for 4 hrs, it was then filtered Using whatmann filter paper and filtered solution was then dried at room Temperature and dry extract was collected.

EVALUATION TEST:

Chemical test for curry leaves:

Test	Observation	Inference
Test for alkaloids: Mayer's regent : To small amount of crude drug add Mayer's reagent (pot. Mercuric Iodide solution)	Yellow ppt	Presence of alkaloids
Drangondroffs test: To small amount of crude drug add dragondroffs reagent.	Orange brown ppt	Presence of alkaloids
Wagner's test: To small amount of crude drug add Wagner's reagent .(Iodine pot.Iodide solution)	Reddish brown ppt	Presence of alkaloids
Hager's test : To small amount of crude drug add haggersreagent.(saturated solution of picric acid)	Yellow ppt	Presence of alkaloids
Test for glycoside Glycoside:Liebermann's test: 2ml of extract + 2ml of CHCl3 + 2ml CH3COOH	Voilet to blue to green coloration	Presence of Glycoside
Antimony trichloride test :	Blue colour	Presence of Glycoside
Tokens test :	Liberation of silver mirror on the walls of blue.	Presence of glycoside
Kellarkillanitest :	Blue colour	Presence of glycoside
Test for flavonoids : Sodium hydroxide test :	Yellow colour	Presence of flavonoids
Shinnodatest : Drug + ethanol .Mix well and filter. To the filterate and Mg turning and add drops of conc. HCL form the site of the test tube observe under white back ground.	Red or voilet colour is produced	Presence of flavonoids
Fecl3 test :Aqueous extract + 5% alcoholic fecl3.	Blue colour	Presence of Flavoinid
Gelatintest : Aqueous extract +gelatin + Nacl.	Milky white colour	Presence of flavonoids
Lead acetate :Aqueous extract + lead acetate.	Precipitate of tannin	Presence of flavonoids
Test for saponins :Powdered plant sample 0.5 gm was boiled by 10 ml of dist. water and 2.5 ml of dist.water and shaken vigorously for a stable persistentfrothing. Frothing was mixed with 3 drops of saturated oil and shaken.	Emulsion forms	Presence of saponins
Test for terpenoids:3ml of extract dissolve in 1ml of chloroform in test Tube and added 1ml of conc. Sulphuric acid in test tube	Red brown colour	Presence of terpenoids



Bioassay

Definition: A bioassay is the "determination of the relative strength of a substance (as a drug) by comparing its effect on a test organism with that of a standard preparation."

Principle: The basic principle of bioassay is to compare the test substance with the International Standard preparation of the same and to find out how much test substance is required to produce the same biological effect, as produced by the standard.

Procedure:

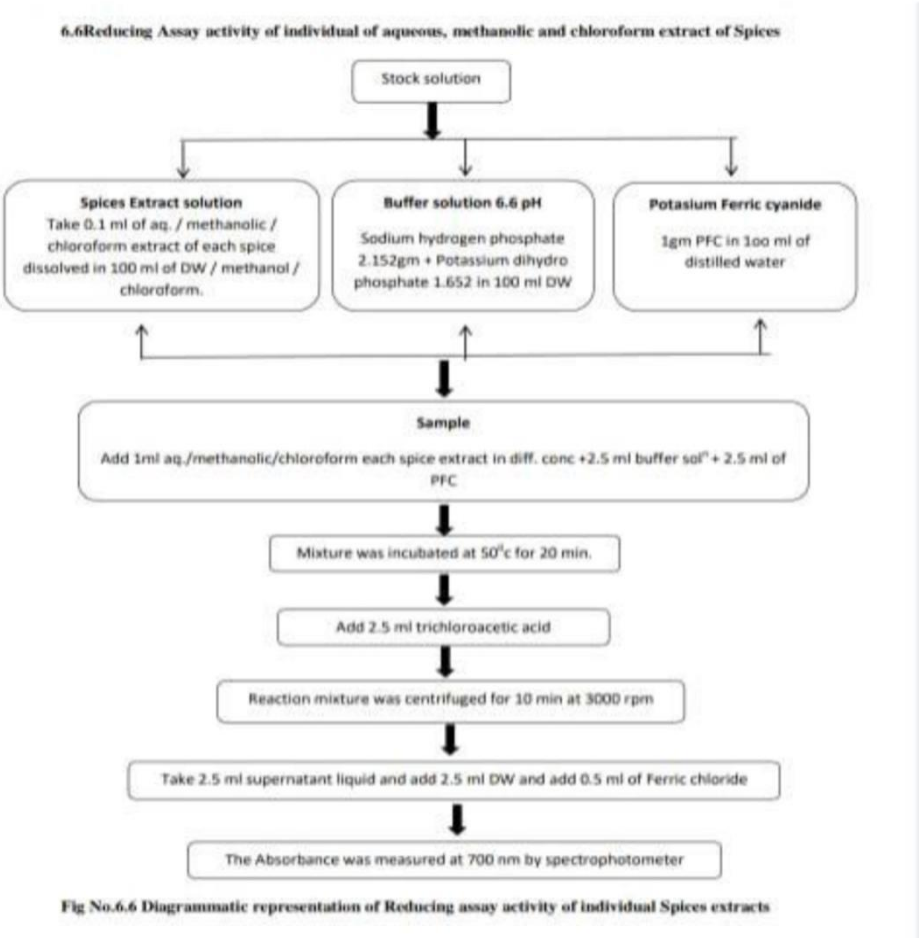


Fig No.6.6 Diagrammatic representation of Reducing assay activity of individual Spices extracts

Observation:

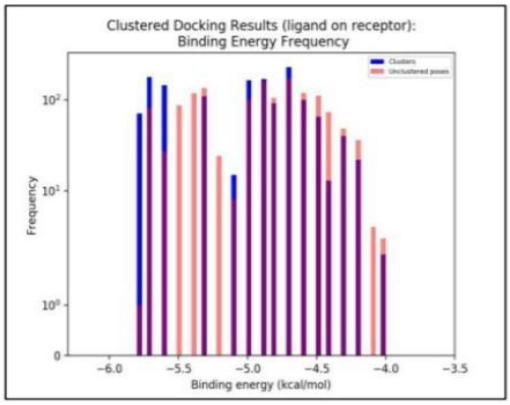
RESULT:

Docking analysis

Docking was performed by an online molecular modeling software Achilles Blind Docking Server to carry out Blind Docking calculation of protein and ligands. Results for Blind Docking to Elemol (mol) on 1ERE (ppdb) RECEPTOR: 1ERE(pdb) LEGAND: Elemol(mol)

1. **(Visual representation of molecules created with 3Dmol)**

BLIND ENERGIES DISTRIBUTION:



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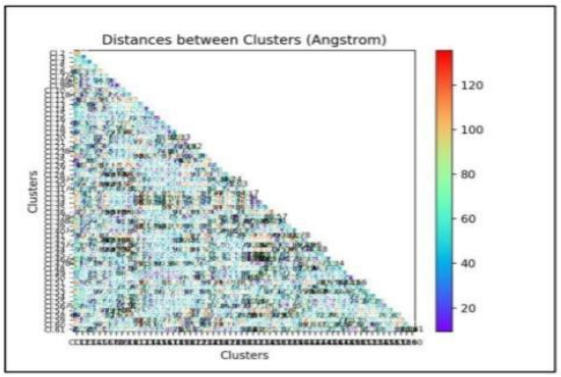
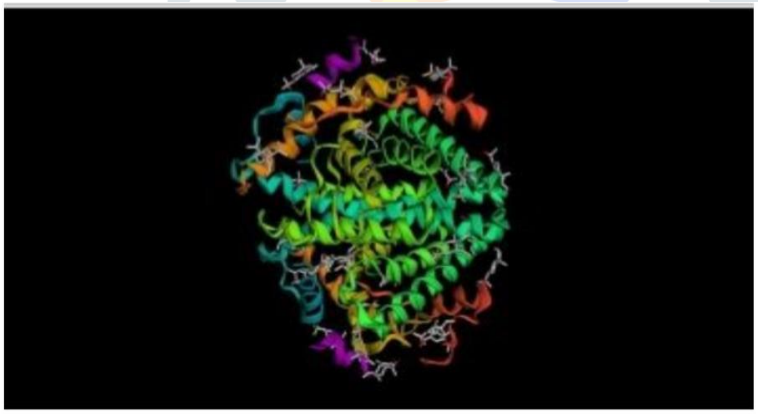


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 70	50	1260	(38.63,22.82,50.25)
2	-5. 70	58	797	(35.00,22.86,83.43)
3	-5. 70	70	587	(10.72,54.98,92.19)
4	-5. 60	76	1038	(57.03,58.32,40.99)
5	-5. 60	69	91	(5.57,56.47,125.16)
6	-5. 30	49	1239	(46.49,30.32,74.42)
7	-5. 30	60	708	(25.47,28.58,59.48)
8	-5. 10	15	872	(24.78,22.29,67.45)
9	-5. 00	29	1080	(65.38,48.48,27.35)
10	-5. 00	15	1186	(48.02,24.23,66.55)

RECEPTOR: 1GWQ(pdb)

LEGAND: ELEMOL(mol)



Visual representation of molecules created with 3Dmol)

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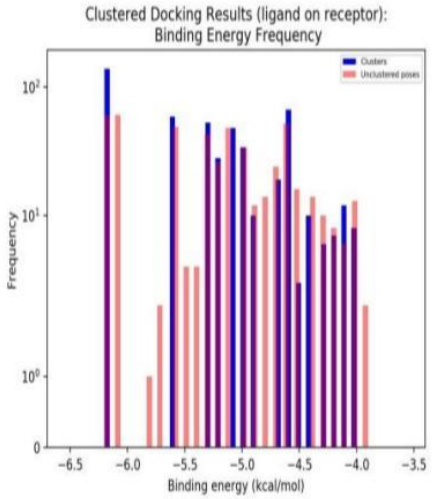

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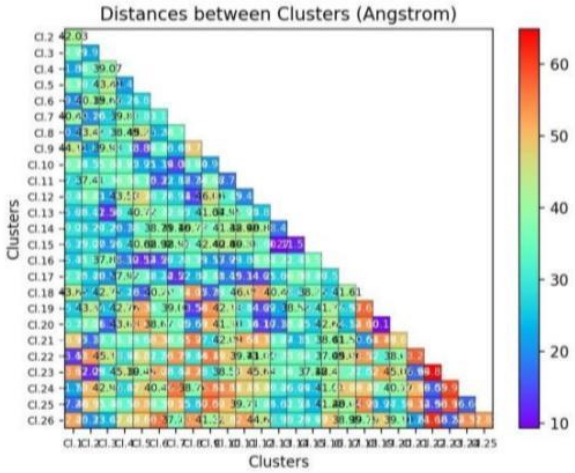
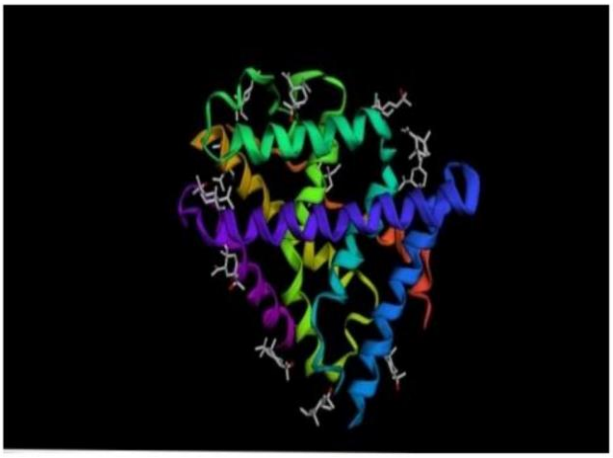


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co Ordinates
1	-6. 20	72	271	(21.25,-11.33,0.00)
2	-6. 20	67	40	(15.73,11.50,34.85)
3	-5. 60	59	205	(11.68,-10.02,33.63)
4	-5. 30	53	165	(16.40,9.92,0.36)
5	-5.20	28	172	(30.68,21.85,10.95)
6	-5. 10	22	440	(38.59,-3.12,5.29)
7	-5. 10	26	187	(34.12,3.39,35.40)
8	-5. 00	34	300	(30.57,-23.35,13.55)
9	-4. 90	10	9	(30.28,24.15,24.64)

RECEPTOR: 1QKM(pdb)

LEGAND: ELEMOL(mol)



Visual representation of molecules created with 3Dmol)

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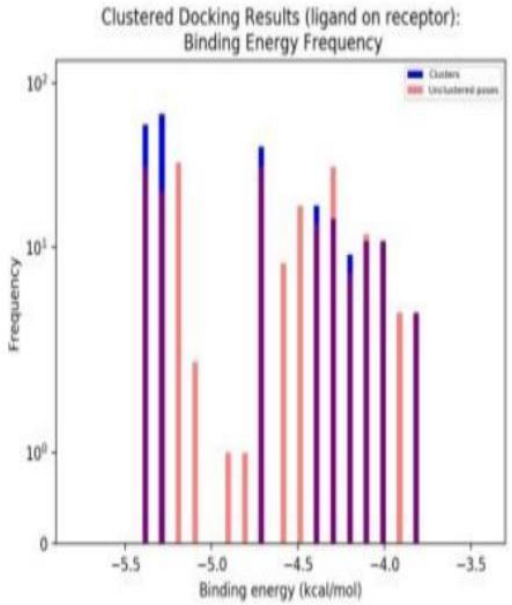

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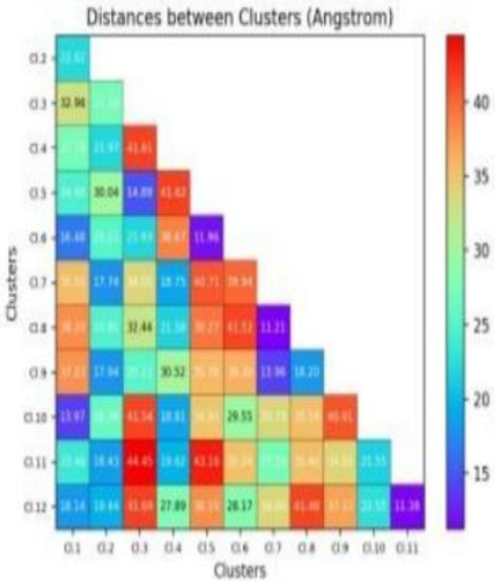
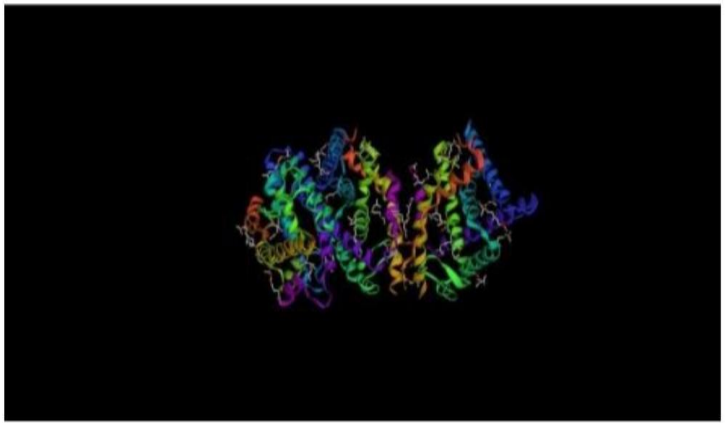


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 40	56	33	(16.36,-2.08,114.07)
2	-5. 30	65	131	(33.46,9.26,106.09)
3	-4. 70	41	54	(46.24,-14.64,108.09
4	-4. 40	18	117	(29.11,19.20,125.20)
5	-4. 30	2	144	(33.03,-20.14,112.19)
6	-4. 30	13	143	(24.39,-14.25,106.38)
7	-4. 20	9	172	(45.21,18.56,115.60)
8	-4. 10	11	181	(49.83,13.22,124.31)
9	-4. 00	7	166	(51.39,10.01,106.46)
10	-4. 00	4	105	(14.85,6.96,124.61)

RECEPTOR: 1R5K (pdb)

LEGAND: GERANYLACETATE (mol)



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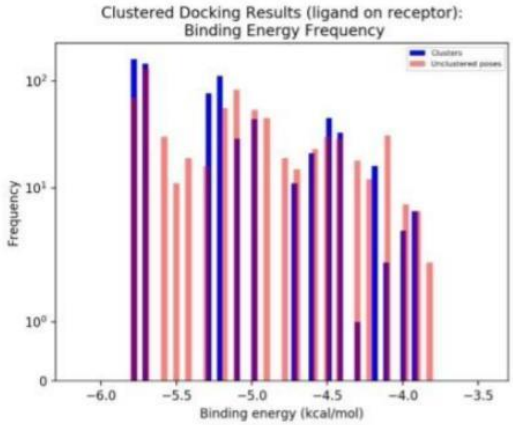

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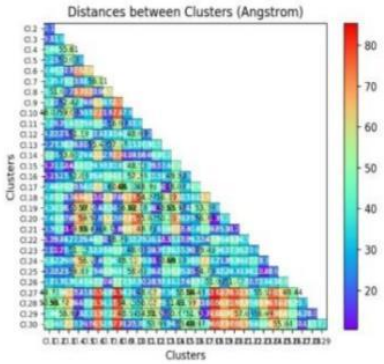

CLUSTER POPULATION:

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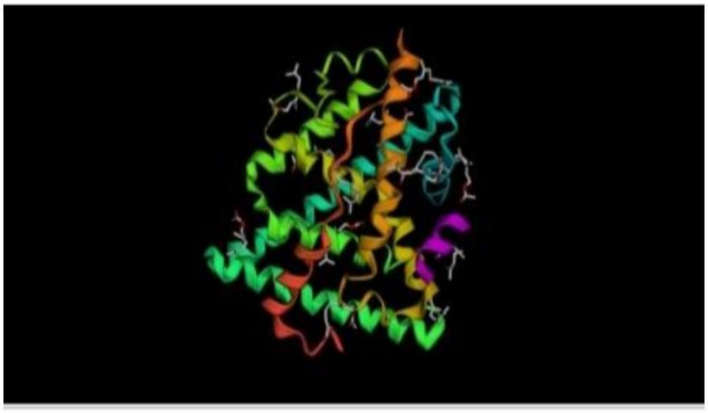
2	-5. 80	69	81	(-9.26,55.16,343.17)
3	-5. 70	64	517	(17.04,46.25,327.99)
4	-5. 70	81	286	(-29.86,20.88,343.82)
5	-5.30	77	197	(-31.78,48.43,338.95)
6	-5. 20	35	620	(29.73,58.41,331.19)
7	-5. 20	77	161	(-11.64,29.16,355.29)
8	-5. 10	29	655	(35.73,43.74,320.61)
9	-5. 00	27	189	(-25.92,56.27,356.31)
10	-5. 00	17	418	(-27.79,29.17,362.49)

RECEPTOR: 1X7R (pdb) LEGAND: GERANYLACETATE (mol)



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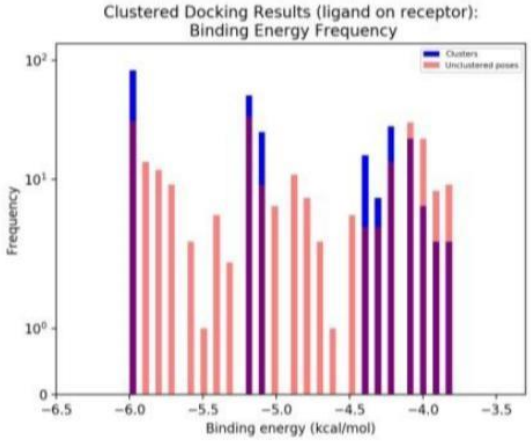

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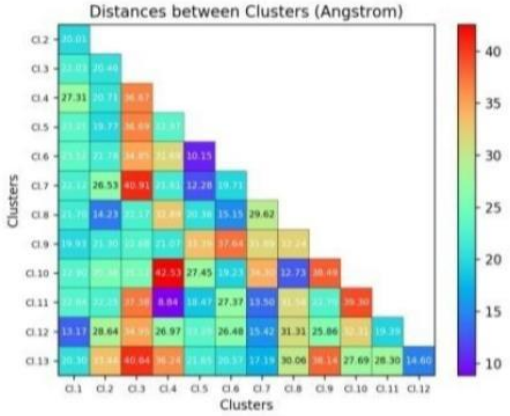
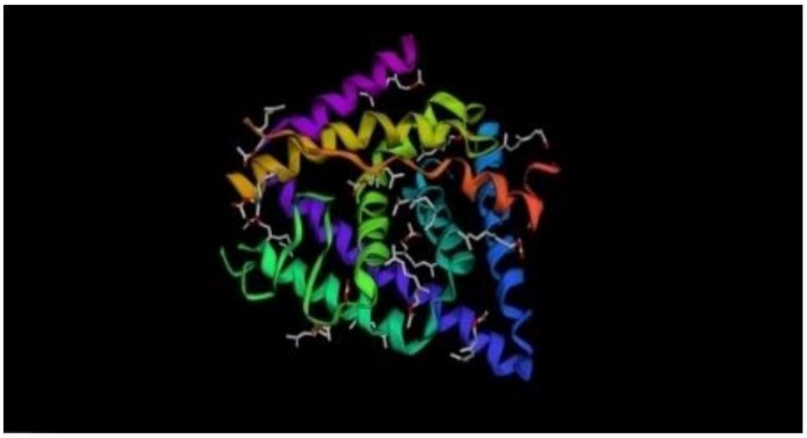


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-6. 00	83	135	(11.76,24.79,13.60)
2	-5. 20	51	193	(29.90,30.91,7.75)
3	-5. 10	25	173	(15.25,33.67,-6.25)
4	-4. 40	16	62	(36.17,12.68,15.34)
5	-4. 30	7	231	(29.30,30.90,27.52)
6	-4. 20	28	106	(24.23,39.67,26.87)
7	-4. 10	7	223	(24.09,20.50,31.46)
8	-4. 10	2	116	(23.61,42.91,22.09)
9	-4. 10	13	55	(21.09,12.87,0.64)
10	-4. 00	6	101	(12.02,47.67,14.35)

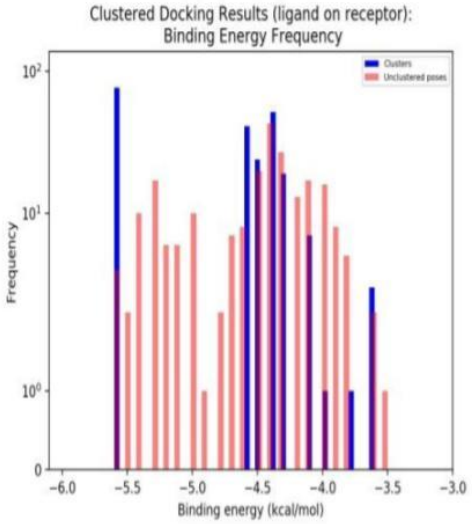
RECEPTOR: 2GIU (pdb)

LEGAND: GERANYL ACETATE (mol)

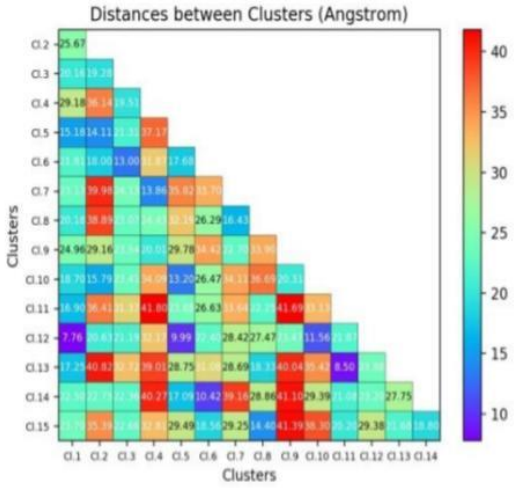


Visual representation of molecules created with 3Dmol)

BLIND ENERGIES DISTRIBUTION:



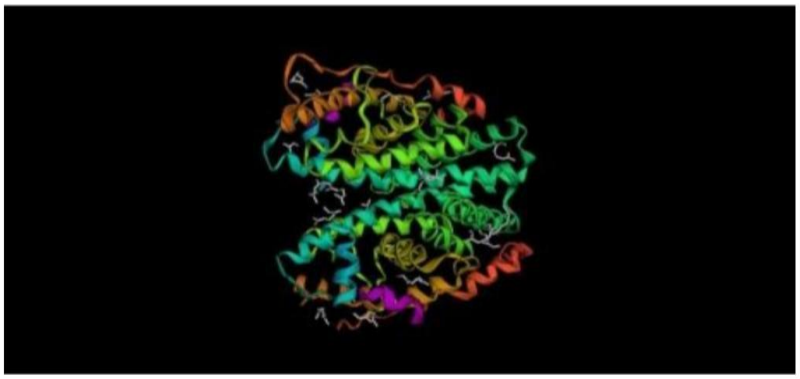
DISTANCE BETWEEN CLUSTERS:



CLUSTER POPULATION:

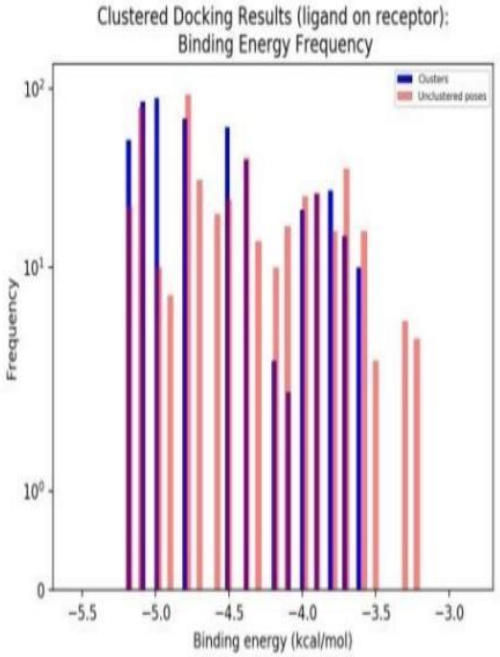
Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 60	77	94	(31.27,8.45,106.15)
2	-4. 60	27	188	(51.15,12.02,121.99)
3	-4. 60	14	184	(37.19-1.26,122.79)
4	-4. 50	24	143	(33.90-19.06,115.52)
5	-4. 40	3	10	(41.49,17.24,113.12)
6	-4. 40	15	116	(34.16,10.40,127.68)
7	-4. 40	12	222	(25.18-13.87,106.08)
8	-4. 40	22	204	(16.05-2.48,113.63)
9	-4. 30	19	0	(47.48-10.37,103.68)
10	-4. 10	2	166	(49.93,9.61,106.43)

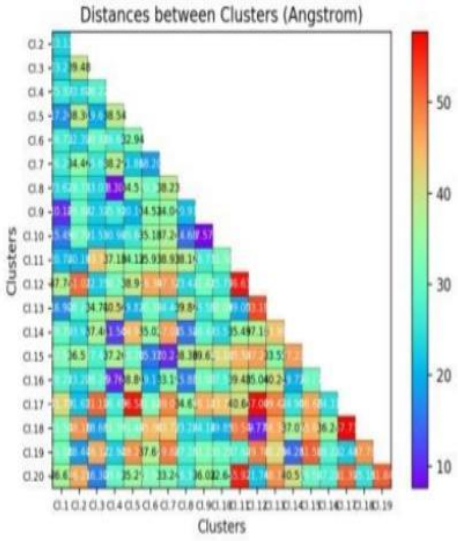
RECEPTOR: 3HLV (pdb) LEGAND: MYRCENE (mol)



Visual representation of molecules created with 3Dmol)

BLIND ENERGIES DISTRIBUTION: DISTANCE BETWEEN CLUSTER:

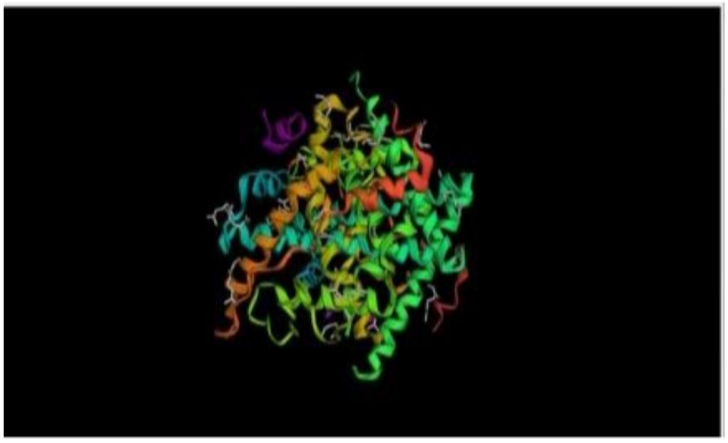




CLUSTER POPULATION:

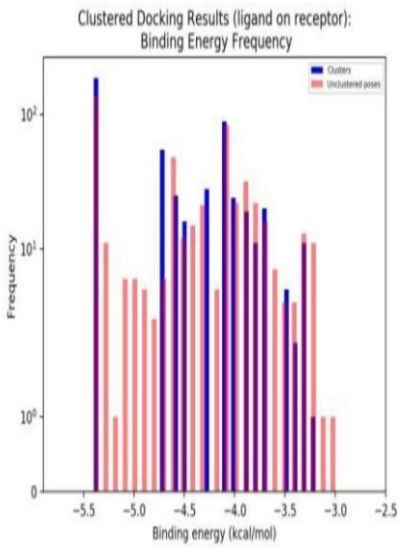
Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 20	52	406	(16.45,8.90,13.82)
2	-5. 10	85	261	(2.95-1.73,29.29)
3	-5. 00	89	127	(15.57,1.10-8.02)
4	-4. 80	68	214	(-7.58,0.99,8.12)
5	-4. 50	21	192	(30.27,6.76,3.70)
6	-4. 50	40	362	(10.66-17.17,15.02)
7	-4. 40	26	438	(27.45-14.36,8.59)
8	-4. 40	14	105	(-4.22,6.20,2.60)
9	-4. 20	3	309	(13.16,16.53,7.95)
10	-4. 10	2	92	(6.45,16.12,4.45)

RECEPTOR: 5DRM (pdb) LEGAND: MYRCENE (mol)

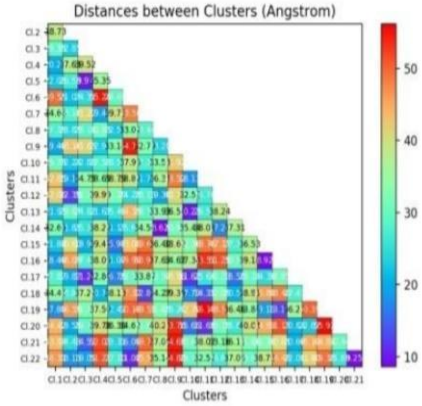


Visual representation of molecules created with 3Dmol)

BLIND ENERGIES DISTRIBUTION:



DISTANCE BETWEEN CLUSTERS

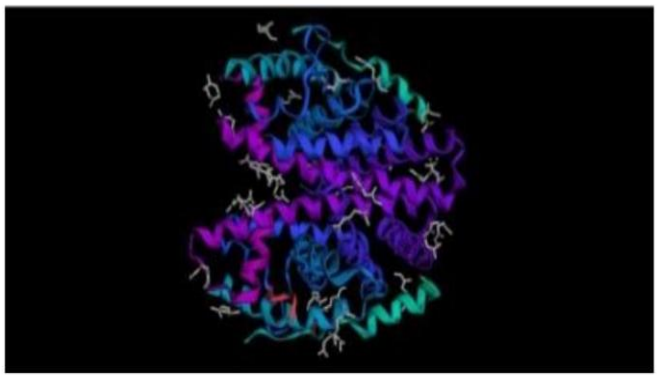


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 40	98	264	(14.91,0.54,8.25)
2	-5. 40	89	90	(2.35,0.59,28.39)
3	-4. 70	55	471	(-9.05,2.34,8.67)
4	-4. 60	25	326	(29.80,7.54,3.62)
5	-4. 50	16	444	(-3.69,-3.73,2.85)
6	-4. 30	28	43	(-16.49,-8.89,28.90)
7	-4. 10	46	180	(29.63,4.85,22.83)
8	-4. 10	43	389	(12.06,-15.57,13.72)
9	-4. 00	24	241	(27.15,-13.96,-3.83)
10	-3. 90	19	159	(6.76,17.57,14.80)

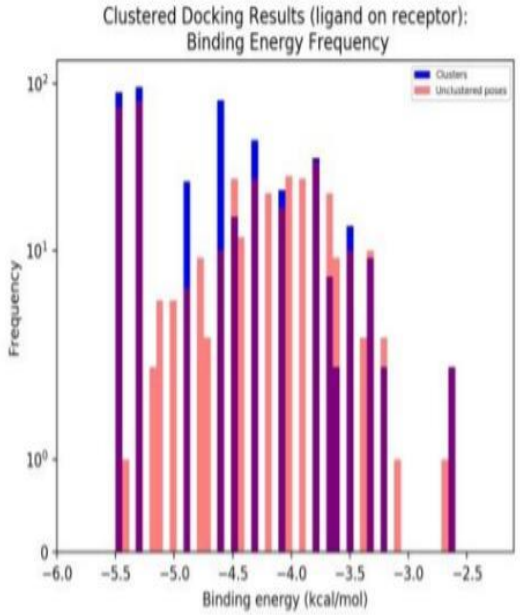
RECEPTOR: 6PIT (pdb)

LEGAND: MYRECENE (mol)

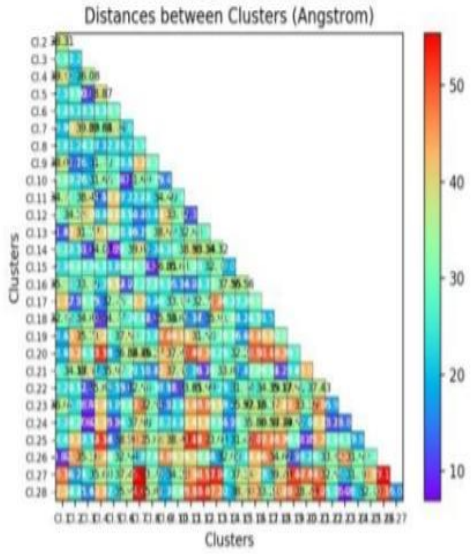


Visual representation of molecules created with 3Dmol) BLIND

ENERGIES DISTRIBUTION:



DISTANCE BETWEEN CLUSTERS

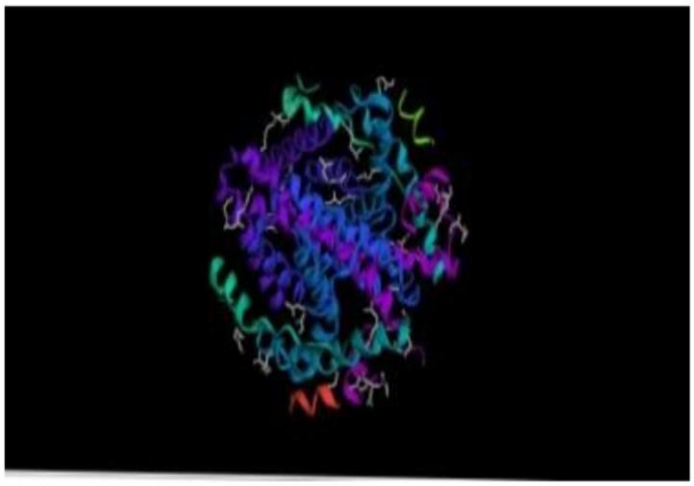


CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 50	89	283	(3.79,-0.74,30.25)
2	-5. 30	96	112	(15.76,-0.50,–6.15)
3	-4. 90	26	192	(–2.32,–4.50,4.30)
4	-4. 60	38	182	(31.88,7.00,4.08)
5	-4. 60	42	419	(-6.30,3.46,10.47)
6	-4. 50	16	138	(17.89,-12.64,13.75)
7	-4. 30	24	224	(23.21,–3.15,33.87)
8	-4. 30	7	278	(15.63,9.56,12.60)
9	-4. 30	15	55	(8.67,–12.29,–5.68)
10	-4. 10	23	152	(13.15,–18.23,7.88)

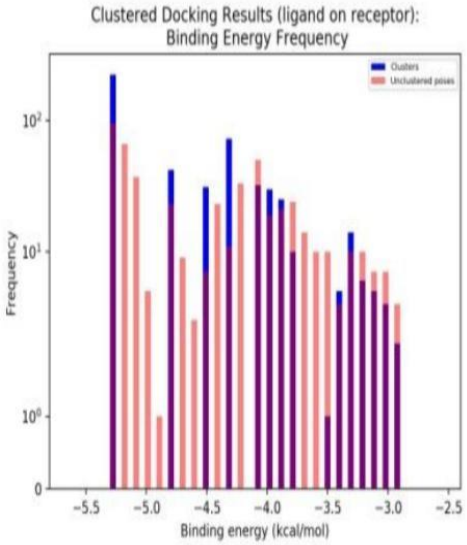
RECEPTOR: 7JHD (pdb)

LEGAND: MYRECENE (mol)



Visual representation of molecules created with 3Dmol)

BLIND ENERGIES DISTRIBUTION:



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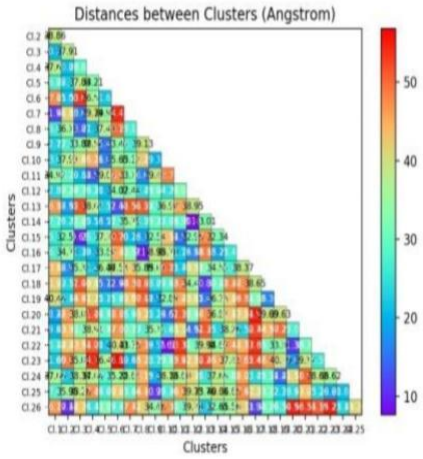

CLUSTER POPULATION:

Sr. No.	Blind energy	Poses in cluster	Best poses	Blinding site co-ordinates
1	-5. 30	110	51	(12.90,–2.81,–2.71)
2	-5. 30	113	278	(0.52,–2.53,33.76)
3	-4. 80	42	127	(-7.30,–2.73,–3.54)
4	-4. 50	31	429	(–12.58,9.64,21.97)
5	-4. 30	73	485	(19.15,-0.02,23.39)
6	-4. 10	9	269	(16.05,5.11,44.17)
7	-4. 10	7	96	(5.44,–11.28,-6.68)
8	-4. 10	16	153	(–9.14,10.21,1.10)
9	-4. 00	30	110	(17.57,–13.82,16.61)
10	-3. 90	17	213	(30.42,–0.07,11.95)

CONCLUSION:

Extracts from Murraya koenigii have shown to be particularly effective against E. As a result, curry leaves may be a viable alternative to antibiotic treatments for the prevention of bacterial infections. CORRECTION: Murraya bacteria, inhibition zone, and antimicrobial properties. koenigii (Murraya) Curry leaves A leafy vegetable from the Rutaceae family is known as koenigii. the numerous noteworthy pharmacological effects of the herb include cardiac and anti-inflammatory effects antidiabetic and cholesterol-lowering properties, antimicrobial, antiulcer Antioxidant properties, cytotoxic effects, antidiarrheal effects, and phagocytic effects. The Murraya koenigii fresh leaves include the following chemical compounds: flammable fuel Stem bark has yielded triterpenes and carbazole alkaloids. and Murraya koenigii roots. Curry leaves hence merit further phytochemical,Pharmacological and clinical research to create a potent natural remedy

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