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Exploring Novel Strategies for Androgen Receptor Activity: via Computational Biology a Therapeutic Interventions in Androgen-Driven Disease (PHASE 1)

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Abstract: Prostate cancer is the most common cancer that impacts men globally, causing a major health issue because of its high occurrence and serious rate of illness and death. It originates in the prostate gland, an important part of the male reproductive system, and it is more likely to occur in individuals over the age of 50. This type of cancer is known to be an androgen-dependent disease as they depend on androgen receptors (AR) for their growth and development. Treatment options for prostate cancer include androgen receptor (AR) antagonistic therapy or combined androgen block therapy. In this study, we applied both ligands-based and receptor-based studies, initially the androgen receptor was retrieved from RCSB PDB, and the PDB ID of the androgen receptor is 1E3G. were receptor protein is further purified on Biovia Discovery Studio and energy is minimized via Swiss Pdb viewer. The receptor protein is further processed for binding pocket detection via Drugrep. In this study, we aim to explore the anticancer properties of natural compounds obtained from the Naturally Occurring Plant-Based Anti-cancerous Compound-Activity-Target database (NPACT). We obtained 242 inhibitor molecules from the NPACT database; these libraries of inhibitor molecules underwent Adsorption Distribution Metabolism Excretion [ADME] analysis to evaluate the drug-likeness properties of the inhibitor After the ADME analysis the number of inhibitor molecules was reduced to 69. Then this inhibitor molecule was subjected to docking analysis on CB-DOCK2, after the binding energy analysis on cb-dock2 we got 4 lead molecules namely APIGENIN (class flavonoid), DAIDZEIN (class flavonoid), LUTEOLIN (class flavonoid) and ALPHA-LAPACHONE (class Polycyclic aromatic natural products). These four molecules were subjected to additional docking analyses using Auto-dock, cb-dock2, Arbuslab, and Swiss dock. Based on the docking study, it was determined that alpha-apache showing more consistence performance in different docking analysis and it is considered as potent inhibitor for androgen receptor.

Keywords: Prostate, Androgen receptor**,** Androgen silencing,Ligand-based designing,

I. INTRODUCTION

Prostate cancer is cancer that occurs in the prostate. The prostate is a small walnut-shaped gland in males that produces the seminal fluid that nourishes and transports sperm Prostate cancer is one of the most common types of cancer. Many prostate cancers grow slowly and are confined to the prostate gland, where they may not cause serious harm. When cancer starts in the prostate, it is called prostate cancer. The prostate is a part of the male reproductive system. All men are at risk for prostate cancer. The most common risk factor is age. Some men are at increased risk for prostate cancer. Prostate cancer is a type of cancer that develops in the prostate gland, which is a part of the male reproductive system. The prostate gland is located just below the bladder and in front of the rectum. While some prostate cancers grow slowly and may not cause significant harm, others can be aggressive and spread quickly to other parts of the body, Risk factors for developing prostate cancer include age, with the risk increasing significantly after the age of 50, and family history of the disease. African American men are also at a higher risk of developing prostate cancer compared to men of other ethnicities.

Symptoms of prostate cancer can vary, and in the early stages, there may be no symptoms at all. However, as the cancer progresses, symptoms may include difficulty urinating, blood in the urine or semen, erectile dysfunction, pain in the hips, back, or chest, and weakness or numbness in the legs or feet. Screening for prostate cancer typically involves a combination of a digital rectal exam

(DRE) and a blood test to measure prostate-specific antigen (PSA) levels. If prostate cancer is suspected based on screening results or symptoms, further diagnostic tests such as a biopsy may be performed to confirm the diagnosis. The incidence of prostate cancer cases detected annually fluctuates due to factors like population demographics, healthcare accessibility, screening protocols, and evolving risk factors. Prostate cancer ranks among the most prevalent cancers diagnosed in men worldwide. To illustrate, the American Cancer Society offers projections on the anticipated number of fresh prostate cancer cases in the United States. Based on their statistics, it was estimated that approximately 248,530 new cases of prostate cancer would be diagnosed in the United States alone in 2022.

Pathophysiology of prostate cancer

The prostate is about the size of a walnut, measuring around 3 centimeters in length and 20 grams in weight. Its job is to generate roughly one-third of the entire seminal fluid. The base of the penis is where the prostate gland is situated in the male pelvis. It is directly in front of the rectum and beneath (inferior) to the bladder (Toivanen, R., & Shen, M. M. et al 2017). The prostate gland requires androgen (testosterone) to function optimally. This is why hormonal therapy (testosterone deprivation) is so effective. Castrate-resistant tumors are thought to generate intracellular androgens (Alukal, J. P., & Lepor, H. 2016). Prostate cancer is an adenocarcinoma as it develops primarily from the glandular part of the organ and shows typical glandular patterns on microscopic examination. The cancer cells grow and begin to multiply, initially spreading to the immediately surrounding prostate tissue and forming a tumor nodule. Such a tumor may grow outside the prostate (extracapsular extension) or may remain localized within the prostate for decades. Prostate cancer commonly metastasizes to the bones and lymph nodes. Metastases to the bone are thought to be partially due to the prostatic venous plexus draining into the vertebral veins. (Leslie SW, Soon-Sutton TL, R I A, et al). The prostate is an organ that produces citrate and accumulates zinc. Prostate cells actively take up zinc thanks to the action of the protein ZIP1. One of zinc's crucial functions is to alter a cell's metabolism to enable the production of citrate, a crucial component of semen. (Mustafa, M., et al.2016).

Risk Factors (Age)

A study of age-specific incidence curves reveals that Prostate cancer risk rises with age, particularly after 50. People 65 years of age or older are diagnosed with prostate cancer in about 60% of cases. Prostate cancer diagnosis in older persons might provide particular difficulties, particularly in the context of cancer therapy (Gann P. H. 2002).

Family history

About 20% of cases of prostate cancer are familial prostate cancers, which are tumors that run in families. A combination of common genes and shared environmental or lifestyle variables leads to the development of this form of prostate cancer. About 5% of occurrences are hereditary prostate cancer, which is a rare form of the disease where the risk is inherited from a relative. Gene alterations, or mutations, that are passed down from one generation to the next within a family cause hereditary prostate cancer. We refer to this as a germline mutation. A person is two to three times more likely to develop prostate cancer than the average person if they have a first-degree relative a parent, sibling, or child who has the disease. Hereditary prostate cancer may be suspected if a family history includes any of the following characteristics or more first-degree relatives with prostate cancer, Prostate cancer in 3 generations on the same side of the family, 2 or more close relatives, such as a parent, sibling, child, grandparent, uncle, or nephew, on the same side of the family diagnosed with prostate cancer before age 55(Bergengren, O., et al 2023).

Genetic Factors

One's risk is increased if a close relative has prostate cancer, indicating a hereditary susceptibility. Because of inherited genetic abnormalities, rare disorders such as Lynch syndrome and hereditary prostate cancer are linked to increased risk of prostate cancer. Prostate cancer risks vary depending on race and ethnicity due to genetic variances. Men of African American descent, for example, have a higher incidence. Treatment choices can be influenced by certain gene expression patterns that indicate the aggressiveness of prostate cancer (Ghayour-Mobarhan, M., et al 2019).

2. AIM

Silencing of androgen receptor protein with the help of chemical compounds that are available in various natural resources.

3. OBJECTIVE

1. Random selection of chemical compounds (ligands).
2. Analysis of compounds
3. Docking of selected compounds with androgen receptor protein
4. Analysis of the best-docked compounds

4.REVIEW OF LITERATURE

1. Nikles, S., et al 2022, studied on Prostate Cancer Diagnosis

Prostate cancer is the most common cancer in men. Diagnosis of prostate cancer poses a significant challenge, due to several different key parameters that need to be evaluated, such as age, history of prostate-specific antigen (PSA), clinical examination, and more recently magnetic resonance imaging (MRI). The current diagnostic pathway for prostate cancer has resulted in overdiagnosis

and overtreatment as well as underdiagnosis and missed diagnoses in many men. Multiparametric MRI (mp-MRI) of the prostate has been identified as a test that could alleviate these diagnostic errors. Before prostate cancer treatment pathological confirmation is mandatory. Prostate biopsy is an invasive procedure with rare but not negligible potential complications. There are several methods of prostate biopsy of which the most common are systemic or planar prostate biopsy and cognitive or targeted MRI-guided prostate biopsy. Multiparametric MRI has demonstrated better accuracy and reproducibility in detecting, locating, and evaluating prostate cancer and also sparing some men unnecessary biopsies. Recent studies have shown a mpMRI benefit for better procedure planning regarding prostate cancer location, extent of disease, and length of the urethra. There are still some challenges ahead, such as ensuring high-quality execution and reporting of mpMRI and ensuring that this diagnostic pathway is cost-effective. According to the latest urological clinical guidelines mpMRI became a fundamental tool in the management of prostate cancer.

2. Handelsman DJ. (2020) studied on Androgen.

androgen, or male sex hormone, is defined as a substance capable of developing and maintaining masculine characteristics in reproductive tissues (notably the genital tract, secondary sexual characteristics, and fertility) and contributing to the anabolic status of somatic tissues. Testosterone together with its potent metabolite, dihydrotestosterone (DHT), are the principal androgens in the circulation of mature male mammals. Testosterone has a characteristic four ring C18 steroid structure and is synthesized mainly by Leydig cells, located in the interstitium of the testis between the seminiferous tubules. Leydig cell secretion creates a very high local concentration of testosterone in the testis as well as a steep downhill concentration gradient into the bloodstream maintaining circulating testosterone levels which exert characteristic androgenic effects on distant androgen sensitive target tissues. The classical biological effects of androgens are primarily mediated by binding to the androgen receptor, a member of the steroid nuclear receptor superfamily encoded by a single gene located on the X chromosome, which then leads to a characteristic patterns of gene expression by regulating the transcription of an array of androgen responsive target genes. This physiological definition of an androgen in the whole animal is now complemented by a biochemical and pharmacological definition of an androgen as a chemical that effectively competes with testosterone binding to the androgen receptor.

3. Lonergan, P. E., et al (2011) studied on antrogen receptor

However, AR differs from other nuclear receptors in this respect and interacts with coactivators in a unique manner. This pocket in the LBD binds preferentially to FxxLF motifs found in the NTD, and interacts poorly with LxxLL motifs commonly found in coactivator. As a result, the hydrophobic pocket within the AR LBD facilitates intramolecular and intermolecular interaction between the AR NTD and its carboxy-terminal domain (CTD), resulting in the dimerization of AR. This NTD/CTD interaction occurs predominately when AR is not bound to DNA. These interactions facilitate the nuclear targeting of AR and AR homodimer formation. Once inside the nucleus, AR binds to specific recognition sequences known as androgen response elements (AREs) in the promoter and enhancer regions of target genes. The AR transcriptional complex is completed by recruitment of coregulators, which ultimately results in modulation of gene expression.

5.MATERIALS AND METHOD

1. **Target Identification and 3D Structure Retrieval**

Define the biological target and understand its role in disease then identify the molecular target, such as a protein or enzyme. Gain insights into the structural characteristics and biological function of the target.

2. **Target Selection and Validation**

Choose a target that is relevant and validated for the disease. Validate the target's draggability and importance using experimental methods. Ensure the target's suitability for small molecule intervention.

3. **Ligand and Structure Database Preparation**

Gather and curate databases of molecular structures of known ligands. Prepare the 3D structure of the target protein using experimental or computational methods.

4. **Virtual Screening of Ligands**

Employ computational algorithms to screen chemical libraries for potential ligands. Dock ligands into the target binding site and assess their binding affinity and interactions. Utilize methods such as molecular docking and molecular dynamics simulations.

5. **Lead Optimization**

Identify promising lead compounds from virtual screening results. Optimize lead compounds to enhance potency, selectivity, and pharmacokinetic properties. Utilize structure-activity relationship (SAR) analysis and combinatorial chemistry for lead optimization.

6. **ADME-Tox Prediction**

Predict the absorption, distribution, metabolism, excretion, and toxicity (ADME-Tox) properties of lead compounds. Assess potential risks and safety profiles to prioritize lead compounds for further development.

7. **Experimental Validation**

Synthesize lead compounds and test their biological activities in vitro. Validate binding affinity, pharmacological effects, and therapeutic potential. Use biochemical assays, cell-based assays, animal studies, and clinical trials for validation.

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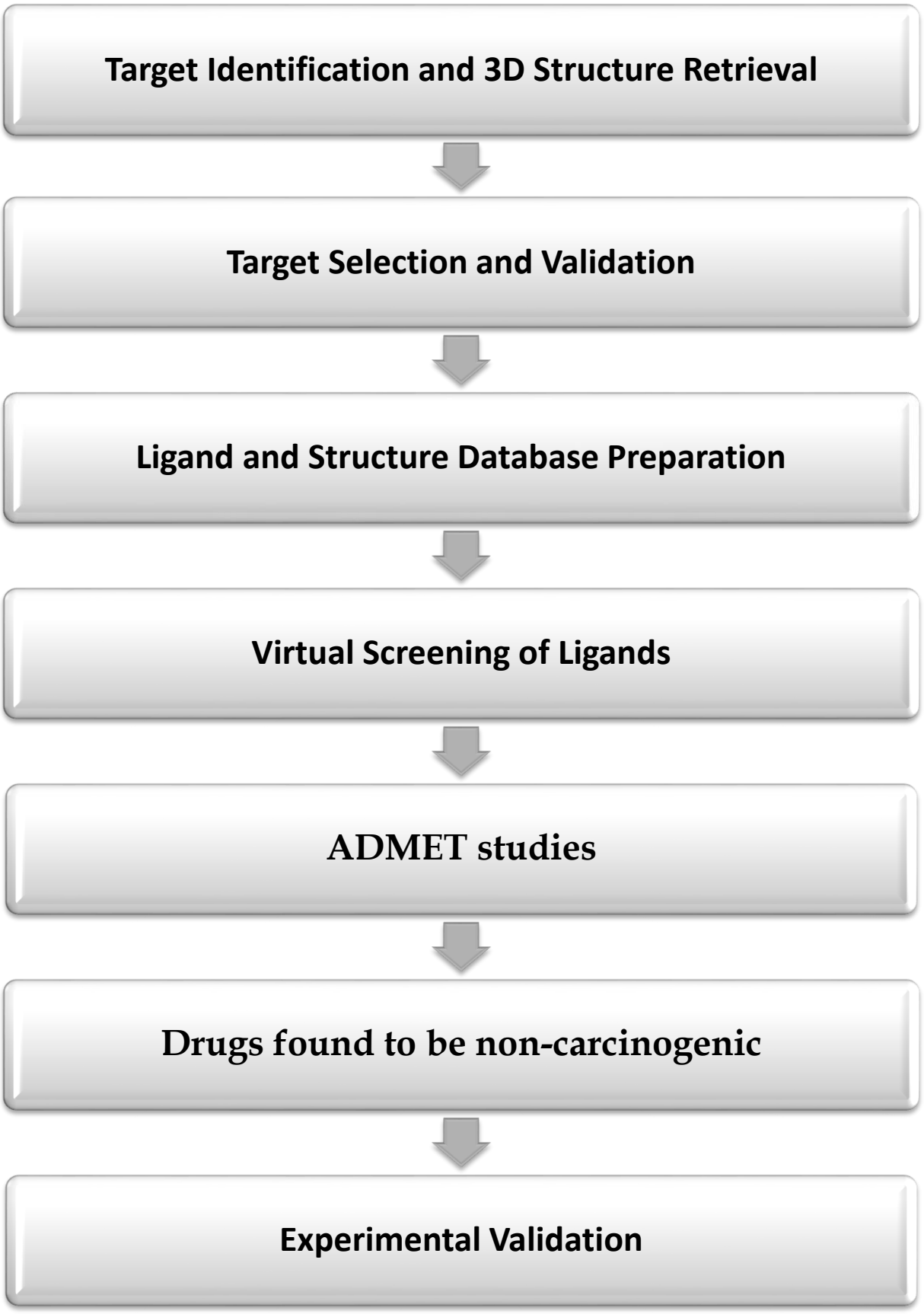

5.RESULT

3D-Structure retrieval of receptor protein (androgen receptor)

The androgen receptor (AR) which is associated with prostate cancer, the crystallographic structure of these proteins was retrieve from protein data bank (PDB). The PDBT ID of the AR is 1E3G, the protein AR contains ONE chains (A) with a resolution of 2.40A. After the retrieval of the proteins from the protein data bank, the proteins went for purification process on Biovia Discovery Studio.

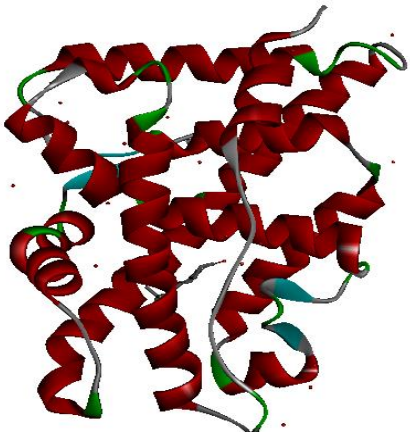

Fig:1 3D Structure of androgen receptor

4 Binding pocket detection via Drugrep

DrugRep is a computer-aided drug discovery online tool for virtual screening of drugs, particularly for drug repurposing. Binding pocket detection refers to the process of identifying and characterizing the three-dimensional structure of binding sites or pockets i.e. X, Y and Z coordinates on proteins where ligands, such as small molecules or other proteins, can bind. These binding pockets play a crucial role in mediating protein-ligand interactions, which are fundamental in various biological processes, including enzymatic reactions, signal transduction, and drug action and it is also very crucial for flexible docking analysis, in this analysis we get different binding coordinates i.e. X=7.5,

Y=18.4 and Z=5.5.

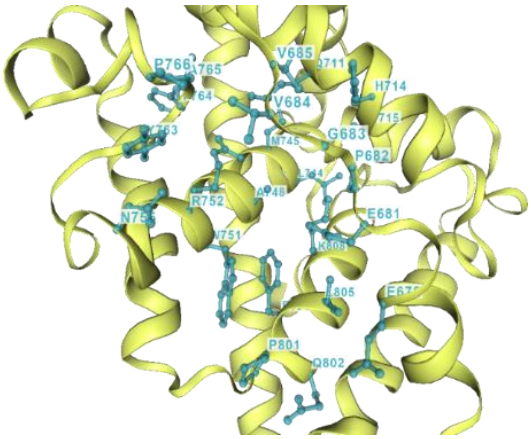

Fig:2 showing different amino acid residues present on androgen receptor

2 Ligand preparation

Computational drug discovery and structure-based drug design both depend on the ligand synthesis stage. It includes the production and optimisation of small molecules (ligands) for computational analyses such as virtual screening, molecular docking, and other targeted at finding possible therapeutic candidates. In this study the Ligands having inhibitory activity against the androgen receptor were randomly taken from Naturally Occurring Plant-Based Anti-cancerous Compound-Activity-Target database (NPACT). Then, after the retrieval of the ligands from the database, screening of the ligands was done to check its drug likeness property by ADME screening and RO5 screening

Table 1: LIST OF INHIBITORS OF ANDROGEN RECEPTOR RETRIEVED FROM NPACT DATABASE

SI.no	NPACT ID	COMPOUND	MOL.FORMULLA	MOL.WT g/mol	SMILE ID
1	NPACT00001	(-) Cycloxanthochymol	C38H50O6	602.800	O1C2=C(C(=O)[C@@]3(C([C@@H](C[C@]2(C3=O)C[C@@H](C1(C)C)CCC(=C)C)CC=C(C)C)(C)C)CC=C(C)C)C(=O)c1cc(O)c(O)cc1
2	NPACT00003	(-) Garcinialiptone A	C38H48O6	602.800	O=C1[C@@]2(C([C@H]3[C@@H]([C@@](C2=O)(C(=O)[C@@]1(C3)C[C@@H](CCC(=C)C)C(=C)C)C(=O)c1cc(O)c(O)cc1)C=C(C)C)(C)C)CC=C(C)C
3	NPACT00007	(+) Garcinialiptone A	C38H50O5	586.8	[C@@H]1([C@@]2(C(=O)[C@@]3(C([C@H]1C[C@@](C3=O)(C2=O)C[C@H](C(=C)C)CCC(=C)C)(C)C)CC=C(C)C)Cc1ccc(c(c1)O)O)C=C(C)C
4	NPACT00009	(2,4-cis and trans)-gigantecinone	$C_{37}H_{66}O_8$	600.900	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCC)[C@H](O)CC[C@H](O)[C@H]1O[C@@H](CC1)CCCCC[C@H]1OC(=O)[C@H](C1)CC(=O)C
5	NPACT00010	(2,4-cis and trans)-squamoxinone	C37H68O7	624.9	O1[C@H](CC[C@@H]1[C@@H](O)CCCCCCCCCCC)[C@H](O)CCCCC[C@H](O)CCCCCC[C@H]1OC(=O)[C@@H](C1)CC(=O)C
6	NPACT00020	(4R,6R)-dihydroxy-4-[10(Z)-heptadecenyl]-2-cyclohexenone	C23H40O3	364.6	O[C@]1(CCCCCCCCC/C=CCCCCCC)C[C@H](O)C(=O)C=C1
7	NPACT00022	1,2,4-trihydroxyheptadec-16-ene	C17H34O3	286.4	O[C@H](CCCCCCCCCCCCC=C)C[C@H](O)CO
8	NPACT00023	1,2,4-trihydroxyheptadec-16-yne	C17H32O3	284.4	O[C@H](CCCCCCCCCCCC#C)C[C@H](O)CO
9	NPACT00024	1,2,4-trihydroxynonadecane	C19H40O3	316.5	O[C@H](CCCCCCCCCCCCCCC)C[C@H](O)CO
10	NPACT00026	1,3-diacetylvilasinin	C30H40O7	512.6	O1[C@H]2[C@@H]3[C@@]([C@@H]4[C@@]([C@@H]2O)(C2=CC[C@H]([C@@]2(CC4)C)c2ccoc2)C)([C@@H](OC(=O)C)C[C@@H](OC(=O)C)[C@]3(C1)C)C
11	NPACT00029	10-Epi-olguine	C18H22O9	382.4	O1[C@@H]([C@@H]1/C=C/[C@@H](OC(=O)C)[C@@H](OC(=O)C)C)[C@@H]1OC(=O)C=C[C@@H]1OC(=O)C
12	NPACT00031	10-Hydroxyasimicin	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCC)CC[C@@H]1[C@H](O)CCCC[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C

13	NPACT00033	10-Hydroxytrilobacin	C37H66O8	638.9	O1[C@@H]([C@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCC)CC[C@@H]1[C@H](O)CCCC[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
14	NPACT00036	12-Deoxyphorbol 13-(9,10-methylene) undecanoate	C32H48O6	528.7	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@@H]2[C@](O)(CC(=C1)CO)C(=O)C(=C2)C)C(=O)CCCCCCC[C@@H]1[C@H](C1)C
15	NPACT00037	12-Deoxyphorbol 20-acetate 13-angelate	C27H36O7	472.6	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@H]2[C@](O)(CC(=C1)COC(=O)C)C(=O)C(=C2)C)C(=O)/C(=CC)/C
16	NPACT00038	12-Deoxyphorbol 20-acetate 13-phenylacetate	C30H36O7	508.6	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@H]2[C@](O)(CC(=C1)COC(=O)C)C(=O)C(=C2)C)C(=O)Cc1ccccc1
17	NPACT00053	1-beta,6-alpha-dihydroxy-4(15)-eudesmene	C15H26O2	238.37	O[C@@H]1[C@@H]2[C@@](CC[C@H]1C(C)C)([C@H](O)CCC2=C)C
18	NPACT00057	1-O-formyl-4'-demethoxy-3',4'-methylenedioxy-methyl rocaglate	C29H26O10	534.5	O1[C@@]2([C@@](O)([C@@H](OC=O)[C@@H]([C@H]2c2ccccc2)C(=O)OC)c2c1cc(OC)cc2OC)c1cc2OCOc2cc1
19	NPACT00068	2-[10(Z)-heptadecenyl]-1,4-hydroquinone	C23H38O2	346.5	Oc1c(CCCCCCCCC/C=CCCCCCC)cc(O)cc1
20	NPACT00069	20-epibryonolic acid	C30H48O3	456.7	Oc1c(CCCCCCCCC/C=CCCCCCC)cc(O)cc1
21	NPACT00070	20-hydroxy-12-deoxyphorbol angelate	C25H34O6	430.5	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@H]2[C@](O)(CC(=C1)CO)C(=O)C(=C2)C)C(=O)/C(=C/C)/C
22	NPACT00071	20-hydroxyresiniferol 9,13, -14-orthophenylacetate	C28H32O6	464.5	O1[C@@]23[C@H]([C@H]4O[C@]1(O[C@]4(C[C@H]2C)C(=C)C)Cc1ccccc1)C=C(C[C@@]1(O)[C@H]3C=C(C1=O)C)CO
23	NPACT00073	22-epicalamistrin	NOT FOUND	NOT FOUND	[C@H]1(O[C@H](CC1)C[C@@H](C[C@H](CCCCCCCCC[CH]CCC1=C[C@H](OC1=O)C)O)OC(=O)C)[C@@H](CCCCCCCCCCCC)O
24	NPACT00085	24-epibrassinolide	C28H48O6	480.7	O1C[C@H]2[C@H]3[C@@]([C@H](CC3)[C@@H]([C@@H](O)[C@H](O)[C@H](C(C)C)C)C)(CC[C@@H]2[C@@]2([C@H](C[C@H](O)[C@H](O)C2)C1=O)C)C
25	NPACT00085	24-epibrassinolide	C37H66O8	638.9	O1C[C@H]2[C@H]3[C@@]([C@H](CC3)[C@@H]([C@@H](O)[C@H](O)[C@H](C(C)C)C)C)(CC[C@@H]2[C@@]

					2([C@H](C[C@H](O)[C@H](O)C2)C1=O)C)C
26	NPACT00089	28-deoxonimbolide	C27H32O6	452.5	O1[C@H]2[C@]([C@@H]([C@@]3([C@H]4[C@H]2OC[C@@]4(C=CC3=O)C)C)CC(=O)OC)(C2=C([C@H](C[C@@H]12)c1ccoc1)C)C
27	NPACT00090	28-homocastasterone	C29H50O5	478.7	OC(CCc1c2c(oc3c(c2=O)c(O)c(c(O)c3)CC=C(C)C)cc(O)c1OC)(C)C
28	NPACT00102	convallatoxin	C29H42O10	550.6	OC12C3C(C4(C(O)(CC3)CC(OC3OC(C(O)C(O)C3O)C)CC4)C=O)CCC1(C(CC2)C1=CC(=O)OC1)C
29	NPACT00104	3,3',4',5,6,7,8-heptamethoxyflavone	C22H24O9	432.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)c(OC)c1c1cc(OC)c(OC)cc1
30	NPACT00109	3,5'-dihydroxythalifaboramine	C39H44N2O9	684.8	O(c1c2c3[C@@H](N(CCc3c(O)c1OC)C)Cc1c2cc(OC)c(O)c1Oc1ccc(C[C@@H]2N(CCc3c2cc(OC)c(OC)c3O)C)cc1)C
31	NPACT00111	3,6-Epidioxy-1,10-bisaboladiene	C15H24O2	236.35	O1O[C@@]2(CC[C@@]1([C@H](CCC=C(C)C)C)C=C2)C
32	NPACT00111	3'-O-Methyl-6-(1,1-dimethylallyl) eriodictyol	C21H22O6	370.4	O1[C@@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1cc(OC)c(O)cc1
33	NPACT00115	3-beta,23,28-trihydroxy-12-oleanene 23-caffeate	NOT FOUND	NOT FOUND	C1C[C@@H]([C@@]([C@H]2[C@]1([C@@H]1[C@@](CC2)([C@]2([C@H](CC1)[C@H]1CC(CC[C@@]1(CC2)CO)(C)C)C)C)C)(C)COC(=O)CCc1ccc(c(c1)O)O)O
34	NPACT00116	3-beta,23,28-trihydroxy-12-oleanene 3-beta-caffeate	NOT FOUND	NOT FOUND	C1C[C@@H]([C@@]([C@H]2[C@]1([C@@H]1[C@@](CC2)([C@]2([C@H](CC1)[C@H]1CC(CC[C@@]1(CC2)CO)(C)C)C)C)C)(C)CO)O[C@@H](O)CCc1cc(c(cc1)O)O
35	NPACT00117	strophanthidin	C23H32O6	404.5	O[C@@]12[C@H]3[C@@H]([C@@]4([C@](O)(CC3)C[C@@H](O)CC4)C=O)CC[C@@]1([C@H](CC2)C1=CC(=O)OC1)C
36	NPACT00122	3-beta-O-(E)-coumaroylbetulin	C39H54O5	602.8	O([C@@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4([C@@H]([C@@H]5[C@@](CC4)(CC[C@H]5C(=C)C)C(=O)O)CC3)C)(CC2)C)(CC1)C)(C)C)C(=O)/C=C/c1ccc(O)cc1
37	NPACT00123	3-beta-O-(E)-feruloylbetulin	NOT FOUND	NOT FOUND	C1[C@@H](CC(C2[C@]1(C1[C@@](CC2)(C2C(CC1)C1[C@@H](CC[C@@]1(CC2)CO)C(=C)C)C)C)C)OC(=O)/C=C/c1ccc(c(c1)OC)O
38	NPACT00124	3-beta-trans-(3,4-dihydroxycinnamoyl-oxy) olean-12-en-28-oic acid	C39H54O6	618.8	O([C@@H]1C([C@H]2[C@@]([C@H]3[C@]([C@]4(C(=CC3)[C@@H]3[C@@](CC4)(CCC(C3)(C)C)C(=O)O)C)(CC

					2)C)(CC1)C)(C)C)C(=O)/C=C/c1cc(O)c(O)cc1
39	NPACT00125	3-beta-trans-feruloyloxy-16-beta-hydroxylup-20(29)-ene	NOT FOUND	NOT FOUND	c1cc(c(cc1/C=CC(=O)O[C@@H]1C([C@H]2[C@](CC1)([C@@H]1[C@@](CC2)([C@]2([C@H](CC1)[C@H]1[C@@H](CC[C@@H]1[C@H](C2)O)C(=C)C)C)C)(C)C)OC)C
40	NPACT00128	3-beta-trans-sinapoyloxylup-20(29)-en-28-ol	NOT FOUND	NOT FOUND	c1c(c(c(cc1/C=C/C(=O)O[C@@H]1C([C@H]2[C@](CC1)([C@@H]1[C@@](CC2)([C@]2([C@H](CC1)[C@H]1[C@@H](CC[C@@]1([CH]C2)O)C(=C)C)C)C)(C)C)OC)C)OC
41	NPACT00129	3'-formyl-2',4',6'-trihydroxy-5'-methyldihydrochalcone	C17H16O5	300.3	Oc1c(C(=O)CCc2ccccc2)c(O)c(c(O)c1C)C=O
42	NPACT00130	3-hydroxy-6'-desmethyl-9-O-methylthalifaboramine	C39H44N2O8	668.8	O(c1c2c3[C@@H](N(CCc3c(O)c1OC)C)Cc1c2cc(OC)c(OC)c1Oc1ccc(C[C@@H]2N(CCc3c2cc(OC)c(O)c3)C)cc1)C
43	NPACT00131	3-hydroxythalifaboramine	C39H44N2O8	668.8	O(c1c2c3[C@@H](N(CCc3c(O)c1OC)C)Cc1c2cc(OC)c(O)c1Oc1ccc(C[C@@H]2N(CCc3c2cc(OC)c(OC)c3)C)cc1)C
44	NPACT00133	convallatoxol	C29H44O10	552.7	O[C@@]12C3C([C@@]4([C@](O)(CC3)C[C@@H](O[C@H]3OC([C@@H](O)C(O)C3O)C)CC4)CO)CC[C@@]1([C@H](CC2)C1=CC(=O)OC1)C
45	NPACT00149	4,4'-O-dimethylellagic acid 3-(2",3"-di-O-acetyl)-alpha-L-rhamnoside	C29H44O11	560.5	O1[C@H]([C@H](O)[C@@H](OC(=O)C)[C@@H](OC(=O)C)[C@@H]1Oc1c2oc(=O)c3c4c2c(cc1OC)c(=O)oc4c(O)c(OC)c3)C
46	NPACT00154	4'-demethoxy-3',4'-methylene-dioxy-methyl rocaglate	C28H26O9	506.5	O1[C@@]2([C@@](O)([C@H](O)[C@@H]([C@H]2c2ccccc2)C(=O)OC)c2c1cc(OC)cc2OC)c1cc2OCOc2cc1
47	NPACT00155	4'-demethyldeoxypodophyllotoxin	C21H20O7	384.4	O1C[C@H]2[C@@H]([C@@H](c3c(C2)cc2OCOc2c3)c2cc(OC)c(O)c(OC)c2)C1=O
48	NPACT00156	4'-demethylpodophyllotoxin	C21H20O8	400.4	O1C[C@H]2[C@@H]([C@@H](c3c([C@@H]2O)cc2OCOc2c3)c2cc(OC)c(O)c(OC)c2)C1=O
49	NPACT00157	4-deoxyannoreticuin	C35H64O6	580.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCC)[C@H](O)CCCCC[C@H](O)CCCCCCC1=C[C@@H](OC1=O)C
50	NPACT00159	4-deoxygigantecin	C37H66O7	622.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCC)[C@H](O)CC[C@H](O)[C@H]1O[C@@H](CC1)CCCCCCCC1=C[C@@H](OC1=O)C

51	NPACT00163	4'-O-methylellagic acid 3-(2",3"-di-O-acetyl)-alpha-L-rhamnoside	C25H22O14	546.4	O1[C@@H]([C@H](O)[C@H](OC(=O)C)[C@@H](OC(=O)C)[C@H]1Oc1c2oc(=O)c3c4c2c(cc1O)c(=O)oc4c(O)c(OC)c3)C
52	NPACT00165	5,4'-Dihydroxy-4",4"-dimethyl-5"-methyl-5"-H-dihydrofuruno [2",3":6,7] flavonone	C20H20O5	340.4	O1[C@@H](C(c2c1cc1O[C@@H](CC(=O)c1c2O)c1ccc(O)cc1)(C)C)C
53	NPACT00170	5,7-dimethoxy-3',4'-methylenedioxyflavanone	C17H16O4	284.31	O1[C@H](CC(=O)c2c1cc(OC)cc2OC)c1ccccc1
54	NPACT00172	5-desmethylnobiletin	C20H20O9	404.4	o1c2c(c(O)c(OC)c(OC)c2OC)c(=O)c(O)c1c1cc(OC)c(OC)cc1
55	NPACT00173	5-desmethylsinensetin	C39H44N2O8	668.8	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1cc(OC)c(OC)cc1
56	NPACT00177	5'-hydroxythalifaboramine	C39H44N2O8	668.8	O(c1c2c3[C@@H](N(CCc3cc1OC)C)Cc1c2cc(OC)c(O)c1Oc1ccc(C[C@@H]2N(CCc3c2cc(OC)c(OC)c3O)C)cc1)C
57	NPACT00181	6-(1,1-Dimethylallyl) eriodictyol	C20H20O6	356.4	O1[C@@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1cc(O)c(O)cc1
58	NPACT00182	6-(1,1-Dimethylallyl) naringenin	C20H20O5	340.4	O1[C@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1ccc(O)cc1
59	NPACT00183	6-(2-Hydroxy-3-methyl-3-butenyl)-8-prenyl-eriodictyol	C25H28O7	440.5	O1[C@@H](CC(=O)c2c1c(c(O)c(c2O)C[C@H](O)C(=C)C)/C=C/C(C)C)c1cc(O)c(O)cc1
60	NPACT00184	6,8-Diprenyleriodictyol	C25H28O6	424.5	O1[C@@H](CC(=O)c2c1c(c(O)c(c2O)/C=C/C(C)C)/C=C/C(C)C)c1cc(O)c(O)cc1
61	NPACT00186	6'-desmethylthalifaboramine	C38H42N2O7	638.7	O(c1c2c3[C@@H](N(CCc3cc1OC)C)Cc1c2cc(OC)c(O)c1Oc1ccc(C[C@@H]2N(CCc3c2cc(OC)c(O)c3)C)cc1)C
62	NPACT00193	6-oxo-pristimerol	NOT FOUND	NOT FOUND	c1c(c(c(c2c1C(C(=CC2=O)C)(C)C)C)O)O
63	NPACT00205	glucostrophanthidin	C30H40O5	480.6 g/mol	O[C@@]12C3C([C@@]4([C@](O)(CC3)C[C@@H](O[C@@H]3OC([C@@H](O)C(O)C3O)CO)CC4)C=O)CC[C@@]1([C@H](CC2)C1=CC(=O)OC1)C
64	NPACT00206	9-alpha-hydroxy-1-beta,10-alpha-epoxyparthenolide	$C_{15}H_{20}O_5$	566.6	O1C2(C1C1OC(=O)C(=C)C1CC(O)C1(OC1CC2)C)C
65	NPACT00207	9-alpha-hydroxyparthenolide	$C_{15}H_{20}O_4$	264.32 g/mol	[C@@H]12CC[C@@]3([C@@H]([C@@H]4[C@H](C[C@@H]([C@@]1(O2)C)O)C(=C)C(=O)O4)O3)C
66	NPACT00208	9-beta-hydroxy-1-beta,10-alpha-epoxyparthenolide	C15H20O5	280.32	O1C2(C1C1OC(=O)C(=C)C1CC(O)C1(OC1CC2)C)C
67	NPACT00209	9-beta-hydroxyparthenolide	C15H20O4	264.32 g/mol	[C@@H]12CC[C@@]3([C@@H]([C@@H]4[C@H](C[C@H]([C@@]1(O2)C)O)C(=C)C(=O)O4)O3)C
68	NPACT00213	Aculeatin A	C26H42O4	418.6 g/mol	[C@]12(C=CC(=O)C=C1)O[C@]1(CC2)C[C@@H](O)C[C@H](O1)CCCCCCCCCCCCC

69	NPACT00214	Aculeatin B	C26H42O4	418.6	O1[C@]2(O[C@H](C[C@@H](O)C2)CCCCCCCCCCCCC)CC[C@]21C=CC(=O)C=C2
70	NPACT00215	Aculeatin E	C24H38O4	390.6	O1[C@@]2(O[C@@H](C[C@H](O)C2)CCCCCCCCCCC)CC[C@@]21C=CC(=O)C=C2
71	NPACT00216	Aculeatin F	C24H38O5	390.6	O1[C@]2(O[C@@H](C[C@@H](O)C2)CCCCCCCCCCC)CC[C@@]21C=CC(=O)C=C2
72	NPACT00217	Aculeatol E	C26H44O5	436.6	O1[C@@]2(O[C@@H](C[C@@H](O)C2)CCCCCCCCCCCCCC)CC[C@]21[C@@H](O)CC(=O)C=C2
73	NPACT00224	Aglafolin	C28H28O8	492.5	O1[C@@]2([C@@](O)([C@H](O)[C@@H]([C@H]2c2ccccc2)C(=O)OC)c2c1cc(OC)cc2OC)c1ccc(OC)cc1
74	NPACT00233	Alpha-Curcumene	C15H22	202.33	[C@@H](CCC=C(C)C)(c1ccc(cc1)C)C
75	NPACT00235	Alpha-Humulene	C15H24	204.35	C1(CC=C(CCC=C(CC=C1)C)C)(C)C
76	NPACT00246	Alvaradoins E	C22H22O9	430.4	O1[C@@H]([C@@H]2c3c(C(=O)c4c2cccc4O)c(O)cc(c3)C)[C@H](O)[C@@H](O)[C@@H](O)[C@@H]1OC(=O)C
77	NPACT00247	Alvaradoins F	C22H22O9	430.4	O1[C@H]([C@H]2c3c(C(=O)c4c2cccc4O)c(O)cc(c3)C)[C@H](O)[C@@H](O)[C@@H](O)[C@H]1OC(=O)C
78	NPACT00257	Amomol A	C27H46O4	434.7	O1[C@](OC)(CC[C@]21C=CC(=O)C=C2)C[C@H](O)CCCCCCCCCCCCCC
79	NPACT00258	Amomol B	C27H46O5	434.7	O1[C@](OC)(CC[C@]21C=CC(=O)C=C2)C[C@H](O)CCCCCCCCCCCCC
80	NPACT00262	Annoglaucin	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@@H](O)CCCCCCCCCC)CC[C@@H]1[C@H](O)CCCC[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
81	NPACT00263	Annoglaxin	C35H62O8	610.9	O1[C@H](CC[C@@H]1[C@H](O)CCC(=O)CCC[C@H](O)CCCCCC1=C[C@@H](OC1=O)C)[C@H](O)C[C@@H](O)CCCCCCCCCC
82	NPACT00264	Annomuricine E	C35H64O8	612.9	O1[C@H](CC[C@H]1[C@H](O)CCCCCCCCCCCC)[C@H](O)CCC[C@@H](O)[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
83	NPACT00266	Annonacin A	C35H64O7	596.9	O1[C@H](CC[C@@H]1[C@@H](O)CCCCCCCCCCCC)[C@H](O)CCCC[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
84	NPACT00267	Annoreticuin-9-one	C35H62O7	594.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCC(=O)CCCC[C@@H](O)CC1=C[C@@H](O

					C1=O)C)[C@H](O)CCCCCCCCCCCC
85	NPACT00270	Apigenin	C15H10O5	270.24	o1c2c(c(=O)cc1c1ccc(O)cc1)c(O)cc(O)c2
86	NPACT00278	Arnidiol	C30H50O2	442.7	O[C@@H]1[C@@]2([C@H]([C@@H]3[C@]([C@]4([C@@H]([C@@]5([C@@H](CC4)C([C@@H](O)CC5)(C)C)CC3)C)(C1)C)[C@@H](C(=C)CC2)C)C
87	NPACT00296	Asitrilobins A			C([C@@H]([C@@H]1CC[C@H]([C@H](CCCCCC[C@@H](CCCCC[C@H](CC2=C[C@@H](OC2=C)C)O)O)O)O1)O)CCCCCCCCCCC
88	NPACT00297	Asitrilobins B	C35H64O7	596.9	O1[C@H](CC[C@H]1[C@@H](O)CCCCCCCCCCCC)[C@H](O)CCCC[C@@H](O)CCCCC[C@H](O)CC1=C[C@H](OC1=O)C
89	NPACT00329	Beta-sitosterol	C29H50O	414.7	O[C@@H]1CC2=CC[C@H]3[C@H]4[C@@]([C@H](CC4)[C@@H](CC[C@H](C(C)C)CC)C)(CC[C@@H]3[C@]2(CC1)C)C
90	NPACT00333	Betulinic acid	C30H48O3	456.7	O[C@@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4([C@@H]([C@@H]5[C@@](CC4)(CC[C@H]5C(=C)C)C(=O)O)CC3)C)(CC2)C)(CC1)C)(C)C
91	NPACT00336	Bisabolene	C15H26O	222.37	O[C@]([C@@H]1CCC(=CC1)C)(CCC=C(C)C)C
92	NPACT00337	Bisabolol	C15H24	204.35	C1(=C(CCC=C(C)C)/C)/CCC(=CC1)C
93	NPACT00357	Bullatetrocin	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCCCCCC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@@H](O)CCCCCC[C@@H](O)[C@@H](O)CC
94	NPACT00390	Caracasine	C21H30O3	330.5g/mol	C(CC(=O)OC)[C@@]1([C@H](C(=C)C)CC[C@]23[C@@H]1CC[C@H](C2)C(=C)C3=O)C
95	NPACT00391	Caracasine acid	C20H28O3	316.4g/mol	C(CC(=O)O)[C@@]1([C@H](C(=C)C)CC[C@]23[C@@H]1CC[C@H](C2)C(=C)C3=O)C
96	NPACT00411	Celastrol	C29H38O4	450.6	OC(=O)[C@]1(C[C@H]2[C@]3([C@](CC[C@]2(CC1)C)(C1=CC=C2C(=CC(=O)C(=C2C)O)[C@@]1(CC3)C)C)C)C
97	NPACT00413	Chamaejasmine	C30H22O10	542.5	O1[C@H]([C@H]([C@H]2[C@@H](Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(=O)c2c1cc(O)cc2O)c1ccc(O)cc1
98	NPACT00417	Chelerythrine	C21H18NO4+	348.4	O1c2cc3c4[n+](cc5c(c4ccc3cc2OC1)ccc(OC)c5OC)C

99	NPACT00425	Cis-4-deoxyannoreticuin	C35H64O6	580.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCCC)[C@H](O)CCCCC[C@H](O)CCCCCCC1=C[C@@H](OC1=O)C
100	NPACT00452	Cucurbitacin F	C30H46O7	518.7	O[C@@H]1[C@@H]([C@@]2([C@@]([C@@H]3[C@@]([C@H]4C(=CC3)C([C@H](O)[C@@H](O)C4)(C)C)(C(=O)C2)C)(C1)C)C)[C@@](O)(C)C(=O)/C=C/C(O)(C)C
101	NPACT00472	Cyclofoveoglin	NOT FOUND	NOT FOUND	c1(cc(cc2c1[C@]1([C@H]3[C@H]([C@](O2)(c2ccc(cc2)OC)[C@]1(O)N(C3=O)CCCCNC(=O)c1ccccc1)c1ccccc1)O)OC)OC
102	NPACT00473	Cycloxanthochymol	C38H50O6	602.8	O1C2=C(C(=O)[C@]3(C([C@H](C[C@@]2(C3=O)C[C@H](C1(C)C)CCC(=C)C)CC=C(C)C)(C)C)CC=C(C)C)C(=O)c1cc(O)c(O)cc1
103	NPACT00476	Daidzein	C15H10O4	254.24	o1c2c(c(=O)c(c3ccc(O)cc3)c1)ccc(O)c2
104	NPACT00495	Deoxypodophyllotoxin	C22H22O7	398.4	NOT FOUND
105	NPACT00496	Desacetyluvaricin	C37H66O6	606.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@@H](O)CCCCCCCCCC)CC[C@@H]1[C@H](O)CCCCCCCCCCCCCC1=C[C@@H](OC1=O)C
106	NPACT00497	Desmethylxanthohumol	C20H20O5	340.4	Oc1c(CC=C(C)C)c(O)cc(O)c1C(=O)/C=C/c1ccc(O)cc1
107	NPACT00499	Diacetylphiladelphicalactone C	NOT FOUND	NOT FOUND	C1(=O)C=C[C@@H]([C@]23[C@]1([C@@H]1[C@@H](C[C@H]2O3)[C@H]2[C@](CC1)([C@H]([C@H](C2)OC(=O)C)[C@@]([C@@H]1OC(=O)[C@@H]([C@@](C1)(O)C)C)(C)O)C)C)OC(=O)C
108	NPACT00512	Diphyllin	C21H16O7	380.3	O1Cc2c(c(c3c(c2O)cc(OC)c(OC)c3)c2cc3OCOc3cc2)C1=O
109	NPACT00518	Dysosmarol	C20H24O7	376.4	O1[C@H]([C@@H]([C@@H](C1)[C@H](O)c1cc(OC)cc(O)c1)CO)c1cc(OC)c(O)cc1
110	NPACT00521	Ellagic acid	C14H6O8	302.19	o1c2c3c4c(cc(O)c(O)c4oc(=O)c3cc(O)c2O)c1=O
111	NPACT00536	convalloside	C35H52O15	712.8	OC12C3C(C4(C(O)(CC3)CC(OC3OC(C(OC5OC(C(O)C(O)C5O)CO)C(O)C3O)C)CC4)C=O)CCC1(C(CC2)C1=CC(=O)OC1)C
112	NPACT00565	Escobarine A	C20H26O4	330.4	O1[C@@]2([C@H]3[C@@H]([C@@]4([C@H](C(CCC4)(C)C)C[C@@H]3O)C)CC(=O)[C@]12C#C)C=O
113	NPACT00566	Escobarine B	C20H28O4	332.4	O1[C@@]2([C@H]3[C@@H]([C@@]4([C@H](C(CCC4)(C)C)C[C@@H]3O)C)CC(=O)[C@]12C#C)CO

114	NPACT00583	Foveoglin A	NOT FOUND	NOT FOUND	c1(cc(cc2c1[C@@]1([C@@H]([C@H]([C@](O2)([C@@H]1O)c1ccc(cc1)OC)C(=O)NCCCCNC(=O)c1ccccc1)c1ccccc1)O)OC)OC
115	NPACT00584	Foveoglin B	NOT FOUND	NOT FOUND	1(cc(cc2c1[C@@]1([C@@H]([C@H]([C@](O2)([C@@H]1O)c1ccc(cc1)OC)C(=O)NCCCCNC(=O)c1ccccc1)c1ccccc1)O)OC)OC
116	NPACT00591	Gallic acid	C7H6O5	170.12	Oc1c(O)cc(cc1O)C(=O)O
117	NPACT00592	Gamma-Tocopherol	C28H48O2	416.7	O1[C@](CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)(CCc2c1c(c(c(O)c2)C)C)C
118	NPACT00596	Garcinialiptone B	C38H48O6	600.8	O1C2=C(C(=O)[C@]3(C([C@H](C[C@@]2(C3=O)C[C@H]([C@@H]1C=C(C)C)C(=C)C)CC=C(C)C)(C)C)CC=C(C)C)C(=O)c1cc(O)c(O)cc1
119	NPACT00597	Garcinialiptone C	C38H50O6	602.8	O=C1[C@]2(C([C@H](C[C@]1(C(=C(C2=O)CC=C(C)C)O)CC=C(C)C)C[C@H](CCC(=C)C)C(=C)C)(C)C)C(=O)c1cc(O)c(O)cc
120	NPACT00598	Garcinialiptone D	C38H50O6	602.8	O=C1[C@@]2(C([C@@H](C[C@]1(C(=C(C2=O)CC=C(C)C)O)CC=C(C)C)C[C@@H](CCC(=C)C)C(=C)C)(C)C)C(=O)c1cc(O)c(O)cc1
121	NPACT00624	Glacins A	C35H64O7	596.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCC)[C@H](O)CCCC[C@H](O)CCCCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
122	NPACT00625	Glacins B	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)CCCC[C@H](O)[C@@H](O)CCCCCCCCCC)CC[C@@H]1[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
123	NPACT00634	Goniotetracin	C37H68O7	624.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCCCCCCC)[C@H](O)CC[C@H](O)CCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
124	NPACT00635	Goniothalamicin	C35H64O7	596.9	O1[C@H](CC[C@H]1[C@@H](O)CCCCCCCCCCCCCC)[C@H](O)CC[C@@H](O)CCCCC[C@H](O)CC1=C[C@H](OC1=O)C
125	NPACT00662	Hiravanone	C26H30O6	438.5	O1[C@H](CC(=O)c2c1c(c(O)c(c2O)CC=C(C)C)CC=C(C)C)c1cc(OC)c(O)cc1
126	NPACT00665	Honokiol	C18H18O2	266.3	Oc1c(c2cc(c(O)cc2)CC=C)cc(CC=C)cc1
127	NPACT00668	Indole-3-carboxylaldehyde	C9H7NO	145.16	O=Cc1c2c([nH]c1)cccc2
128	NPACT00670	Isobonducellin	C17H14O4	282.29	O1C/C(=C/c2ccc(OC)cc2)/C(=O)c2c1cc(O)cc2

129	NPACT00674	Isofoveoglin	NOT FOUND	NOT FOUND	c1(cc(cc2c1[C@@]1([C@H]([C@@H]([C@](O2)([C@@H]1O)c1ccc(cc1)OC)c1ccccc1)C(=O)NCCCCNC(=O)c1ccccc1)O)OC)OC
130	NPACT00679	Isorhamnetin 3-O-beta-D-glucopyranoside	C22H22O13	478.4	O1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(OC)c(O)cc1)CO
131	NPACT00685	Isoxanthochymol	C38H50O6	602.8	O1C2=C(C(=O)[C@]3(C([C@H](C[C@@]2(C3=O)C[C@H](C1(C)C)CC=C(C)C)CC=C(C)C)(C)C)CC=C(C)C)C(=O)c1cc(O)c(O)cc1
132	NPACT00686	Ixocarpalactone A	C28H40O8	504.6	O1[C@@]23[C@]([C@@H]4[C@@H]([C@H]5[C@@]([C@@H]([C@H](O)C5)[C@@](O)([C@@H](O)[C@@H]5OC(=O)[C@@H]([C@H]5C)C)C)(CC4)C)C[C@@H]12)(C)C(=O)C=C[C@@H]3O
133	NPACT00687	Jacaranone	C9H10O4	182.1	O[C@]1(CC(=O)OC)C=CC(=O)C=C1
134	NPACT00698	Kaempferol 3-O-beta-D-glucopyranoside	C21H20O11	432.4	O1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c(oc2c(c1=O)c(O)ccc2)c1ccc(O)cc1)CO
135	NPACT00712	Limocitrin 3,5,7,4'-tetramethyl ether	C21H22O8	402.4	o1c2c(c(=O)c(OC)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2OC
136	NPACT00717	Lobatosides B			NOT FOUND
137	NPACT00718	Lobatosides C	C58H90O25	1187.3	NOT FOUND
138	NPACT00719	Lobatosides D	C64H100O30	1349.5	NOT FOUND
139	NPACT00720	Lobatosides E	C65H102O31	1379.5	NOT FOUND
140	NPACT00721	Longimicins A	C37H66O7	622.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCCCCC)CC[C@@H]1[C@H](O)CC[C@H](O)CCCCCCCC1=C[C@@H](OC1=O)C
141	NPACT00722	Longimicins B	C35H62O7	594.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCCCCC)CC[C@@H]1[C@H](O)CCCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
142	NPACT00723	Longimicins C	C35H62O7	594.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCC[C@@H](O)CC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@H](O)CCCCCCCCCCCCCC
143	NPACT00724	Longimicins D	C37H66O7	622.3	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCC[C@@H](O)CC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@H](O)CCCCCCCCCCCCCC
144	NPACT00729	Luteolin	C15H10O6	286.24	o1c2c(c(=O)cc1c1cc(O)c(O)cc1)c(O)cc(O)c2

145	NPACT00763	Melianin B	C41H58O9	694.9	O([C@H]1[C@@]2([C@@H]([C@@]3([C@H](C([C@H](OC(=O)c4ccccc4)C[C@@H]3OC(=O)C)(C)C)C1)C)CC[C@@]1(C2=CC[C@H]1[C@H]1C[C@@H](O)[C@H](O)C(OC1)(C)C)C)C)C(=O)C
146	NPACT00764	Melianin C	C37H48O8	620.8	O([C@H]1[C@@]2([C@@H]([C@@]3([C@H](C([C@H](OC(=O)c4ccccc4)C[C@@H]3OC(=O)C)(C)C)C1)C)CC[C@@]1(C2=CC[C@H]1[C@@H]1CC(=O)OC1)C)C)C(=O)C
147	NPACT00766	Meliavolkinin	C35H42O7	574.7	O1[C@H]2[C@@H]3[C@@]([C@@H]4[C@@]([C@@H]2O)(C2=CC[C@H]([C@@]2(CC4)C)c2ccoc2)C)([C@@H](OC(=O)c2ccccc2)C[C@@H](OC(=O)C)[C@]3(C1)C)C
148	NPACT00772	Methyl gallate	C8H8O5	184.1	Oc1cc(cc(O)c1O)C(=O)OC
149	NPACT00780	Mosin B	C35H62O7	594.9	O1[C@H](CC[C@@H]1[C@H](O)CCCCCC(=O)CCCC[C@@H](O)CC1=C[C@@H](OC1=O)C)[C@@H](O)CCCCCCCCCCCC
150	NPACT00781	Mosin C	C35H62O7	594.9	O1[C@@H](CC[C@@H]1[C@H](O)CCCCCC(=O)CCCC[C@@H](O)CC1=C[C@@H](OC1=O)C)[C@@H](O)CCCCCCCCCCCC
151	NPACT00782	Mosinone A	C37H64O7	620.9	O1[C@H](CC[C@@H]1[C@H](O)CC/C=CCCCCCCCCCC)[C@H](O)CCCCCC(=O)CCCC[C@H]1OC(=O)[C@@H](C1)CC(=O)C
152	NPACT00785	Muricapentocin	C35H64O8	612.9	O1[C@H](CC[C@H]1[C@H](O)CCCCCCCCCCCC)[C@H](O)CC[C@H](O)CCC[C@@H](O)CCC[C@@H](O)CC1=C[C@H](OC1=O)C
153	NPACT00786	Muricatetrocin C	C35H64O7	596.9	O1[C@@H](CC[C@H]1CCCCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C)[C@@H](O)CC[C@@H](O)[C@@H](O)CCCCCCCCCCCC
154	NPACT00787	Muricoreacin	C35H64O9	628.9	O1[C@@H](CC[C@H]1C[C@@H](O)C[C@@H](O)CCC[C@@H](O)CC1=C[C@@H](OC1=O)C)[C@@H](O)CC[C@H](O)[C@H](O)CCCCCCCCCCCC
155	NPACT00788	Murihexocin C	C35H64O9	628.9	O1[C@@H](CC[C@H]1CCC[C@@H](O)[C@H](O)CC[C@@H](O)CC1=C[C@@H](OC1=O)C)[C@@H](O)CC[C@H](O)[C@H](O)CCCCCCCCCCCC
156	NPACT00790	Myricetin	C19H38N2O2	326.5	OC(=O)[C@]1([C@H](CCC1)CCCCCCCC)CCCCCNN

157	NPACT00791	Myricetin 3-O-alpha-rhamnoside	C21H20O12	464.4	O1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1cc(O)c(O)c(O)c1)C
158	NPACT00792	Myricetin 3-O-beta-glucuronide	C21H18O14	494.4	O1[C@@H](Oc2c(oc3c(c2=O)c(O)cc(O)c3)c2cc(O)c(O)c(O)c2)[C@H](O)[C@@H](O)[C@H](O)[C@H]1C(=O)O
159	NPACT00813	Nerolidol	C15H26O	222.37	O[C@](CC/C=C(/CCC=C(C)C)C)(C)C=C
160	NPACT00815	Nimbolide	C27H30O7	466.5	O1[C@H]2[C@@]([C@@H]([C@@]3([C@@H]4[C@@H]2OC(=O)[C@@]4(C=CC3=O)C)C)CC(=O)OC)(C2=C([C@@H](C[C@@H]12)c1ccoc1)C)C
161	NPACT00817	Nobiletin	C21H22O8	402.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)cc1c1cc(OC)c(OC)cc1
162	NPACT00831	Oleanolic acid	C30H48O3	456.7	O[C@@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4(C(=CC3)[C@H]3[C@@](CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
163	NPACT00841	Panduratin A	C26H30O4	406.5	O=C([C@@H]1[C@@H](C(=CC[C@H]1c1ccccc1)C)CC=C(C)C)c1c(O)cc(OC)cc1O
164	NPACT00843	Parthenolid-9-one	NOT FOUND	NOT FOUND	C1=C(C(=O)C[C@@H]2[C@@H]([C@H]3[C@@](CC1)(O3)C)OC(=O)C2)C
165	NPACT00859	Philadelphicalactone A	C28H40O7	488.6	O1[C@@]23[C@]([C@@H]4[C@H]([C@H]5[C@@]([C@](O)(CC5)[C@@](O)([C@H]5OC(=O)[C@@H]([C@H](C5)C)C)C)(CC4)C)C[C@@H]12)(C)C(=O)C=C[C@@H]3O
166	NPACT00860	Philadelphicalactone C	NOT FOUND	NOT FOUND	C1(=O)C=C[C@@H]([C@]23[C@]1([C@@H]1[C@@H](C[C@H]2O3)[C@H]2[C@](CC1)([C@H]([C@H](C2)O)[C@@]([C@@H]1OC(=O)[C@@H]([C@@](C1)(O)C)C)(C)O)C)C)O
167	NPACT00861	Philadelphicalactone D	NOT FOUND	NOT FOUND	C1(=O)C=CC[C@]2([C@]1([C@@H]1[C@@H]([C@H]3[C@@H]2O3)[C@H]2[C@](CC1)([C@H](CC2)[C@@]([C@@H]1OC(=O)[C@@H]([C@@](C1)(O)C)C)(C)O)C)C)O
168	NPACT00864	Phyllamyricin C	NOT FOUND	NOT FOUND	c1(c(c(cc2c1cc1COC(=O)c1c2c1ccc2c(c1)OCO2)OC)OC)OC
169	NPACT00873	Podophyllotoxone	C22H20O8	412.4	O1C[C@H]2[C@@H]([C@@H](c3c(C2=O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
170	NPACT00880	Pristimerin	C30H40O4	464.6	O(C(=O)[C@]1(C[C@H]2[C@]3([C@](CC[C@]2(CC1)C)(C1=CC=C2C(=CC(=O)C(=C2C)O)[C@@]1(CC3)C)C)C)C)C

171	NPACT00888	Purpuracenin	C23H26O10	462.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)c(OC)c1c1c(OC)cc(OC)c(OC)c1
172	NPACT00889	Purpurediolin	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@H](O)CCCCCCCCCCCCC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@@H](O)CCC[C@@H](O)[C@@H](O)CCCCC
173	NPACT00890	Purpurenin	C37H66O8	638.9	O1[C@@H]([C@@H]2O[C@H](CC2)[C@@H](O)CCCC[C@@H](O)CCCCC)CC[C@@H]1[C@H](O)CCCC[C@H](O)CCCCCCCC1=C[C@@H](OC1=O)C
174	NPACT00892	Quercetin 3,5,7,3',4'-pentamethyl ether	C20H20O7	372.4	o1c2c(c(=O)c(OC)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2
175	NPACT00893	Quercetin 3,7,3',4'-tetramethyl ether	C19H18O7	358.3	o1c(c2cc(OC)c(OC)cc2)c(OC)c(=O)c2c1cc(OC)cc2O
176	NPACT00897	Reissantins A	C33H39NO11	625.7	O1[C@@]23[C@]([C@@H](OC(=O)c4ccccc4)[C@@H](OC(=O)C)[C@H]([C@H]2OC(=O)c2cn(c(=O)cc2)C)C1(C)C)([C@@H](OC(=O)C)CC[C@@]3(O)C)C
177	NPACT00898	Reissantins B	C40H43NO13	745.8	O1[C@@]23[C@]([C@@H](OC(=O)c4ccccc4)[C@@H](OC(=O)C)[C@H]([C@H]2OC(=O)c2cn(c(=O)cc2)C)C1(C)C)([C@@H](OC(=O)C)[C@@H](OC(=O)c1ccccc1)C[C@@]3(O)C)C
178	NPACT00899	Reissantins D	C24H32O8	448.5	O1[C@@]23[C@]([C@@H](OC(=O)c4ccccc4)[C@@H](O)[C@H]([C@H]2O)C1(C)C)([C@@H](OC(=O)C)CC[C@@]3(O)C)C
179	NPACT00900	Reissantins E	C26H34O9	490.5	O1[C@@]23[C@]([C@@H](OC(=O)c4ccccc4)[C@@H](OC(=O)C)[C@H]([C@H]2O)C1(C)C)([C@@H](OC(=O)C)CC[C@@]3(O)C)C
180	NPACT00904	Resiniferol 20-(4-hydroxy-3-methoxyphenylacetate) 9,13,14-ortho-phenylacetate	C37H40O9	628.7	O1[C@@]23[C@H]([C@H]4O[C@]1(O[C@]4(C[C@H]2C)C(=C)C)Cc1ccccc1)C=C(C[C@@]1(O)[C@@H]3C=C(C1=O)C)COC(=O)Cc1cc(OC)c(O)cc1
181	NPACT00923	rollidecin A	C37H66O8	638.9	O1[C@H]([C@@H]2O[C@H](CC2)CCCCCCC[C@@H](O)CC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@H](O)CC[C@@H](O)[C@@H](O)CCCCCCCCCC
182	NPACT00924	Rollidecin B	C37H66O8	638.9	O1[C@H]([C@@H]2O[C@H](CC2)CCCCCCC[C@@H](O)CC2=C[C@@H](OC2=O)C)CC[C@@H]1[C@H](O)CC[C

					@@H](O)[C@@H](O)CCCCCCCCCCC
183	NPACT00925	Rollinecins A	C37H68O7	624.9	O1[C@@H](CC[C@@H]1[C@@H](O)CCCCCCCCCCCC)[C@H](O)CC[C@H](O)CCCCCCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
184	NPACT00926	Rollinecins B	C37H68O7	624.9	O1[C@@H](CC[C@@H]1[C@@H](O)CCCCCCCCCCCC)[C@H](O)CC[C@@H](O)CCCCCCCCC[C@@H](O)CC1=C[C@@H](OC1=O)C
185	NPACT00932	S-allylcysteine	C6H11NO2S	161.2	S(C[C@H](N)C(=O)O)CC=C
186	NPACT00933	S-allylmercaptocysteine	C5H9NOS2	163.3	S(SCC=C)CC(=O)N
187	NPACT00944	Secofoveogline	NOT FOUND	NOT FOUND	c1(cc(cc(c1C(=O)[C@@H]([C@@H](C(=O)c1ccc(cc1)OC)c1ccccc1)C(=O)NCCCCNC(=O)c1ccccc1)O)OC)OC
188	NPACT00946	Silvestrol	C34H38O13	654.7	O1[C@@]2([C@@](O)([C@H](O)[C@@H]([C@H]2c2ccccc2)C(=O)OC)c2c1cc(O[C@@H]1O[C@H](CO[C@H]1OC)[C@H](O)CO)cc2OC)c1ccc(OC)cc1
189	NPACT00965	Syriacusins A	C13H12O4	232.2	O(c1c2c(cc(c1O)C)ccc(O)c2C=O)C
190	NPACT00967	Tangeretin	C20H20O7	372.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)cc1c1ccc(OC)cc1
191	NPACT00973	Tetra-o-methylisoscutellarein	C18H16O5	312.3	o1c2c(c(OC)cc(OC)c2)c(=O)cc1c1ccc(OC)cc1
192	NPACT00974	Tetra-o-methylscutellarein	C19H18O6	342.3	o1c2c(c(OC)c(OC)c(OC)c2)c(=O)cc1c1ccc(OC)cc1
193	NPACT00977	Tiliroside	C30H26O13	594.5	O1[C@@H]([C@@H](O)[C@H](O)[C@@H](O)[C@@H]1Oc1c(oc2c(c1=O)c(O)cc(O)c2)c1ccc(O)cc1)COC(=O)/C=C/c1ccc(O)cc1
194	NPACT01002	Uvaribonin	C39H70O8	667	O1[C@H](CC[C@@H]1[C@H](O)CCCCCCCCCCCC)[C@H](OC(=O)C)C[C@H](O)CCCCCCCCC[C@H](O)CCC1=C[C@H](OC1=O)C
195	NPACT01005	Vinblastine	C46H58N4O9	811	O([C@@H]1[C@]2([C@@H]3N(CC[C@@]43[C@@H](N(c3c4cc(c(OC)c3)[C@]3(C[C@H]4C[C@](O)(CN(C4)CCc4c3[nH]c3c4cccc3)CC)C(=O)OC)C)[C@@]1(O)C(=O)OC)CC=C2)CC)C(=O)C
196	NPACT01012	Wedelolactone	C16H10O7	314.25	o1c2c(c3c1cc(O)c(O)c3)c(=O)oc1c2c(O)cc(OC)c1
197	NPACT01018	Withaferin A	C28H38O6	470.6	O1[C@@]23[C@]([C@@H]4[C@H]([C@H]5[C@@]([C@H](CC5)[C@@H]([C@@H]5OC(=O)C(=C(C5)C)CO)C)(CC4)C)C[C@@H]12)(C)C(=O)C=C[C@@H]3O

198	NPACT01020	Withaphysacarpin	C28H40O7	488.6	O1[C@@]23[C@]([C@@H]4[C@H]([C@H]5[C@@]([C@H]([C@@H](O)C5)[C@@](O)([C@@H]5OC(=O)[C@@H]([C@H](C5)C)C)C)(CC4)C)C[C@@H]12)(C)C(=O)C=C[C@@H]3O
199	NPACT01023	Xanthochymol	C38H50O6	602.8	O=C1[C@]2(C([C@H](C[C@]1(C[C@@H](CCC(=C)C)C(=C)C)C(=O)/C(=C(/O)c1cc(O)c(O)cc1)/C2=O)CC=C(C)C)(C)C)CC=C(C)C
200	NPACT01024	Xanthohumol	C21H22O5	354.4	O(c1c(c(O)c(CC=C(C)C)c(O)c1)C(=O)/C=C/c1ccc(O)cc1)C
201	NPACT01039	(-)-usnic acid	C18H16O7	244.3	O1C2=CC(=C(C(=O)[C@]2(c2c1c(c(O)c(c2O)C)C(=O)C)C)C(=O)C)O
202	NPACT01054	(S)-5-hydroxy-7,4'-dimethoxyflavanone	C17H16O5	300.3	O1C(CC(=O)c2c1cc(OC)cc2O)c1ccc(OC)cc1
203	NPACT01065	2-(1-hydroxyethyl) naphtho[2,3-b] furan-4,9-quinone	C14H10O4	242.2	o1c2c(cc1C(O)C)C(=O)c1c(C2=O)cccc1
204	NPACT01073	2-acetylnaphtho[2,3-b]furan-4,9-quinone	NOT FOUND	NOT FOUND	c1(=C)c2c(c(=C)c3c1[CH][C](O3)C(=O)C)cccc2
205	NPACT01082	3-o-(cis-p-coumaroyl)-alphitolic acid	C40H56O6	632.9	O(C1C(C2[C@@](C3C(C4(C(C5C(CC4)(CCC5C(=C)C)C(=O)O)(CC3)C)C)(CC2)C)(CC1O)C)(C)C)C(=O)/C=Cc1ccc(O)cc1
206	NPACT01083	3-o-(cis-p-coumaroyl)-maslinic acid	C39H54O6	618.8	O(C1C(C2C(C3C(C4(C(=CC3)C3C(CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1O)C)(C)C)C(=O)/C=Cc1ccc(O)cc1
207	NPACT01086	toxicarioside M	NOT FOUND	NOT FOUND	C1CC(C[C@@]2(C1(C1C(CC2)[C@@]2([C@](CC1)([C@H](CC2)C1=CC(=O)OC1)C)O)O)O)O[C@H]1O[C@@H](C)[C@@H]([C@H]([C@@H]1O)O)O
208	NPACT01108	9-Aminocamptothecin	C20H17N3O4	363.4	O1Cc2c([C@@](O)(CC)C1=O)cc1n(Cc3c1nc1c(c3)c(N)ccc1)c2=O
209	NPACT01122	alpha-lapachone	C15H14O3	242.2	O1C(CCC2=C1C(=O)c1c(C2=O)cccc1)(C)C
210	NPACT01127	alphitolic acid	C30H46O4	470.7	O[C@@H]1C(C2[C@@](C3[C@]([C@]4(C(=CC3)C3[C@@](CC4)(CC[C@H]3C(=C)C)C(=O)O)C)(CC2)C)(C[C@H]1O)C)(C)C
211	NPACT01129	Andrographolide	C20H30O5	350.4	O[C@H]1[C@]([C@@H]2[C@]([C@@H](C(=C)CC2)C/C=C/2[C@H](O)COC2=O)(CC1)C)(CO)C
212	NPACT01145	beta-caryophyllene oxide	C15H24O	220.3	O1[C@]2([C@H]1CCC(=C)[C@@H]1[C@H](C(C1)(C)C)CC2)C

213	NPACT01148	betulonic acid	C30H46O3	454.7	OC(=O)C12[C@@H]([C@@H]3[C@]([C@]4([C@@H]([C@@]5([C@@H](CC4)C(C(=O)CC5)(C)C)C)CC3)C)(CC1)C)[C@@H](CC2)C(=C)C
214	NPACT01174	cis-3-O-p-Hydroxycinnamoyl Ursolic Acid	C39H54O5	602.8	O([C@@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4(C(=CC3)[C@H]3[C@@](CC4)(CC[C@H]([C@@H]3C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C(=O)/C=Cc1ccc(O)cc1
215	NPACT01176	colubrinic acid	C30H46O4	470.7	O[C@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4([C@@H]([C@@H]5[C@@](CC4)(CC[C@H]5C(=C)C)C(=O)O)CC3)C)(CC2)C)([C@@H]1C=O)C)(C)C
216	NPACT01187	dehydro-iso-alpha-lapachone	C15H12O3	240.25	O1C(CC2=C1C(=O)c1c(C2=O)cccc1)C(=C)C
217	NPACT01211	Fumarprotocetraric acid	C22H16O12	472.4	O1c2c(OC(=O)c3c1c(c(O)cc3C)C=O)c(c(O)c(c2C)C(=O)O)COC(=O)/C=C/C(=O)O
218	NPACT01213	gamma-caryophyllene	C15H24	204.3	C1(C2C(C1)C(=C)CCC=C(CC2)C)(C)C
219	NPACT01227	Hispidulin	C16H12O6	300.26	o1c2c(c(O)c(OC)c(O)c2)c(=O)cc1c1ccc(O)cc1
220	NPACT01263	Membranacin	C37H66O6	606.9	O1[C@@H]([C@@H]2O[C@@H](CC2)[C@@H](O)CCCCCCCCCCC)CC[C@H]1[C@H](O)CCCCCCCCCCCCC1=C[C@@H](OC1=O)C
221	NPACT01284	Neoxanthin	C40H56O4	600.9	O1[C@@]2([C@]1(C[C@@H](O)CC2(C)C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C=C1C(C[C@H](O)C[C@]1(O)C)(C)C)C)C)/C)/C
222	NPACT01286	oleanonic acid	C30H46O3	454.7	O=C1C([C@H]2[C@@]([C@@H]3[C@]([C@]4(C(=CC3)[C@H]3[C@@](CC4)(CCC(C3)(C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C
223	NPACT01302	Psychotrine	C28H40O10	536.6	O(c1cc2C3N(CC(C(C3)CC3=NCCc4c3cc(OC)c(OC)c4)CC)CCc2cc1OC)C
224	NPACT01324	3-O-beta-D-xylopyranosylstrophanthidin	C28H40O10	536.6	O[C@@]12[C@H]3[C@@H]([C@@]4([C@](O)(CC3)C[C@@H](OC3OCC(O)C(O)C3O)CC4)C=O)CC[C@@]1([C@H](CC2)C1=CC(=O)OC1)C
225	NPACT01351	trans-3-O-p-Hydroxycinnamoyl Ursolic Acid	C39H54O5	602.8	O([C@@H]1C([C@H]2[C@@]([C@@H]3[C@]([C@]4(C(=CC3)[C@H]3[C@@](CC4)(CC[C@H]([C@@H]3C)C)C(=O)O)C)(CC2)C)(CC1)C)(C)C)C(=O)/C=C/c1ccc(O)cc1
226	NPACT01357	Tubulosine	C29H37N3O3	475.6	O(c1cc2[C@H]3N(C[C@@H]([C@H](C3)C[C@H]3NCCc4c3[nH]c3c4cc(O)cc3)CC)CCc2cc1OC)C

227	NPACT01386	zizyberenalic acid	C30H44O3	452.7	OC(=O)[C@]12C(C3[C@]([C@]4(C([C@@]5([C@@H](CC4)C(C=C5C=O)(C)C)C)CC3)C)(CC1)C)[C@@H](CC2)C(=C)C
228	NPACT01408	12-Acetoxy-5-hydroxynerolidol	C17H28O4	296.4	O[C@](C[C@@H](O)/C=C(/CC/C=C(/COC(=O)C)C)C)(C)C=C
229	NPACT01445	(1S,5S,6R,7S,9R,10S)-5-Methylbutanoyloxy-1,4,9-trihydroxy-2-oxoxanth-11-en-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[C@H]1O)C(=C)C(=O)O2)OC(=O)C(C)CC)(O)C(=O)CC(C)O)C
230	NPACT01446	9-Oxo-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(CC1=O)C(=C)C(=O)O2)OC(=O)C(C)CC)(C(=O)/C=C/C)O)C
231	NPACT01450	3-o-(trans-p-coumaroyl)-maslinic acid	NOT FOUND	NOT FOUND	C1C(C(C(C2C1(C1C(CC2)(C2(C(=CC1)[C@H]1C(CC2)(C(=O)O)CCC(C1)(C)C)C)C)(C)C)CC1C(CCC(C1)/C=C/C(=O)O)O)O
232	NPACT01453	(1S,5S,6R,7R,8S,10S)-5-Angeloyloxy-1,8-dihydroxy-2-oxoxantha-3,11-dien-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([C@H]([CH]1)O)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
233	NPACT01460	(1S,5S,6R,7S,10R)-1-Hydroxy-4-methoxy-5-methylbutanoyloxy-2,9-dioxoxanth-11-en-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[CH]1)C(=C)C(=O)O2)OC(=O)C(CC)C)(O)C(=O)CC(C)OC)C
234	NPACT01467	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-angelate	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([CH][C@H]1O)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
235	NPACT01479	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[C@H]1O)C(=C)C(=O)O2)OC(=O)C(C)CC)(O)C(=O)/C=C/C)C
236	NPACT01481	(1S,5S,6R,7S,10S)-5-Angeloyloxy-1-hydroxy-2-oxoxantha-3,11-dien-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([CH][CH]1)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
237	NPACT01486	2-alpha, 3-alpha, 19-beta, 23-beta-tetrahydroxyurs-12-en-28-oic acid	NOT FOUND	NOT FOUND	C1[C@@H]([C@@H]([C@@](C2[C@]1(C1[C@@](CC2)([C@]2(C(=CC1)C1[C@@](CC2)(CC[C@@H]([C@@]1(C)O)C)C(=O)O)C)C)(C)CO)O)O
238	NPACT01488	3-o-(trans-p-coumaroyl)-alphitolic acid	NOT FOUND	NOT FOUND	C1C(C(C(C2C1(C1C(CC2)(C2(C(CC1)C1C(CC2)(CCC1C(=C)C)C(=O)O)C)C)(C)C)CC1C(CCC(C1)/C=C/C(=O)O)O)O
239	NPACT01494	(8'S)-neochrome	NOT FOUND	NOT FOUND	C1(C[C@H](C[C@](C1=C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(C)/[C@@H]1C=C2[C@](C[C@H](CC2(C)C)O)(C)O1)C)/C)/C)(C)O)O)(C)C

240	NPACT01495	(8 'R)-neochrome	NOT FOUND	NOT FOUND	C1(C[C@H](C[C@](C1=C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(C)/[C@H]1C=C2[C@](C[C@H](CC2(C)C)O)(C)O1)C)/C)/C)(C)O)O)(C)C
241	NPACT01543	9'-(o-methyl) protocetraric acid	NOT FOUND	NOT FOUND	C1(=O)Oc2c(Oc3c(c(cc(c13)C)O)C=O)c(c(c(c2COC)O)C(=O)O)C
242	NPACT01565	1',2',3',4'-tetradehydrotubulosine	NOT FOUND	NOT FOUND	CC[C@H]1CN2CCc3cc(OC)c(OC)cc3[C@H]2C[C@H]1C[C]1[N][CH][CH]c2c1[nH]c1ccc(O)cc21

1 CB-DOCK2 DOCKING

Pharmaceutical and biological research commonly employs protein-ligand blind docking as a technique to examine the binding sites and poses of ligands and receptors. Now that CB-Dock2 is available, researchers all around the world are using it. Thanks to the knowledge-based docking engine of CB-Dock2, it is possible to anticipate binding poses and identify binding sites more accurately than state-of-the-art approaches. It is an online docking site. Online docking, also known as web-based docking, is a computational method that allows users to perform molecular docking studies remotely through a web interface. It enables researchers to access docking tools and resources without the need for installing specialized software or running complex calculations locally. The bioinformatics community will find this highly automated server to be an effective and user-friendly tool due to its interactive and straightforward input and output web interfaces (Liu, Y., & Cao, Y. 2024).

The screen compounds were successfully docked on cb-dock2 and the and ligands having binding energy less than or equal to 10 (Kcal/Mol) were taken as potent molecules for androgen receptor. From this docking analysis we get four potent molecules for androgen receptor.

Table:2 CB-D0CK2 DOCKING RESULT

S.NO	NAME OF COMPOUND	BINDING AFFINITY(Kcal/Mol)
1	10-EPI-OLGUINE	-7.8
2	12-DEOXYPHORBOL 20-ACETATE 13-ANGELATE	-7.4
3	1-BETA,6-ALPHA-DIHYDROXY-4(15)-EUDESMENE	-7.3
4	20-HYDROXY-12-DEOXYPHORBOL ANGELATE	-7.8
5	20-hydroxyresiniferol 9,13, -14-orthophenylacetate	-7.9
6	28-deoxonimbolide	-8.9
7	28-homocastasterone	-7.8
8	3,6-Epidioxy-1,10-bisaboladiene	-7.4
9	3'-O-Methyl-6-(1,1-dimethylallyl) eriodictyol	-7.3
10	strophanthidin	-7.3
11	3'-formyl-2',4',6'-trihydroxy-5'-methyldihydrochalcone	-8.0
12	4'-demethyldeoxypodophyllotoxin	-7.9
13	4'-demethylpodophyllotoxin	-8.0
14	5,4'-Dihydroxy-4",4"-dimethyl-5"-methyl-5"-H-dihydrofuruno [2",3":6,7] flavonone	-8.8

15	5,7-dimethoxy-3',4'-methylenedioxyflavanone	-7.9
16	5-desmethylnobiletin	-7.3
17	5-desmethylsinensetin	-7.4
18	6-(1,1-Dimethylallyl) eriodictyol	-7.5
19	6-(1,1-Dimethylallyl) naringenin	-8.3
20	6-(2-Hydroxy-3-methyl-3-butenyl)-8-prenyl-eriodictyol	-7.3
21	6-oxo-pristimerol	-8.2
22	9-alpha-hydroxy-1-beta,10-alpha-epoxyparthenolide	-8.1
23	9-alpha-hydroxyparthenolide	-7.4
24	9-beta-hydroxy-1-beta,10-alpha-epoxyparthenolide	-8.0
25	Apigenin	-9.9
26	Cadralazine	-8.5
27	Cadralazine acid	-7.4
28	Chama jasmine	-7.7
29	Daidzein	-9.1
30	Deoxy podophyllotoxin	-7.9
31	Desmethylxanthohumol	-7.7
32	Diphyllin	-7.7
33	Dysosmarol	-7.4
35	Escobarine A	-7.2
36	Escobarine B	-7.5
37	Honokiol	-7.8
38	Isobonducellin	-7.8
39	Limocitrin 3,5,7,4'-tetramethyl ether	-7.3
40	Luteolin	-9.4
41	Nobiletin	-7.0
42	Parthenolid-9-one	-6.4
43	Phyllamyricin C	-7.3
44	Podophyllotoxone	-7.6
45	Purpuracenin	-6.7
46	Quercetin 3,5,7,3',4'-pentamethyl ether	-7.7
47	Quercetin 3,7,3',4'-tetramethyl ether	-7.6
48	Reissantins D	-7.1

49	Syriacusins A	-8.6
50	Tangeretin	-6.5
51	Tetra-o-methylisoscutellarein	-7.9
52	Tetra-o-methylscutellarein	-7.6
53	Wedelolactone	-8.5
54	(-)-usnic acid	-7.9
55	(S)-5-hydroxy-7,4'-dimethoxyflavanone	-7.7
56	2-(1-hydroxyethyl) naphtho[2,3-b] furan-4,9-quinone	-8.7
57	2-acetylnaphtho[2,3-b] furan-4,9-quinone	-8.8
58	9-Aminocamptothecin	-8.5
59	alpha-lapachone	-9.1
60	Andrographolide	-7.3
61	dehydro-iso-alpha-lapachone	-8.6
62	Hispidulin	-7.5
63	(1S,5S,6R,7S,9R,10S)-5-Methylbutanoyloxy-1,4,9-trihydroxy-2-oxoxanth-11-en-6,12-olide	-6.9
64	9-Oxo-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	-6.9
65	(1S,5S,6R,7R,8S,10S)-5-Angeloyloxy-1,8-dihydroxy-2-oxoxantha-3,11-dien-6,12-olide	-7.0
66	(1S,5S,6R,7S,10R)-1-Hydroxy-4-methoxy-5-methylbutanoyloxy-2,9-dioxoxanth-11-en-6,12-olide	-6.7
67	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-angelate	-8.1
68	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	-6.8
69	(1S,5S,6R,7S,10S)-5-Angeloyloxy-1-hydroxy-2-oxoxantha-3,11-dien-6,12-olide	-7.3

After the CB dock2 docking we go for further clarification via auto-dock4.2, swiss dock, argus lab

Table 3: DOCKING ANALYSIS OF ANDROGEN RECEPTOR

SI.NO	COMPOUND NAME	CB-DOCK2	ARGOUS LAB	SWISS DOCK	AUTO DOCK	MEAN SCORE
1	APIGENIN	-9.9	-8.52469	-8.60	-6.99	-8.50
2	DAIDZEIN	-9.1	-11.8971	-7.99	-6.92	-8.97
3	LUTEOLIN	-9.4	-8.64328	-8.38	-6.32	-8.18
4	ALPHA-LAPACHONE	-9.1	-10.3193	-7.62	-7.43	-8.61

Inhibitors Auto Dock Binding Affinity, with androgen receptor

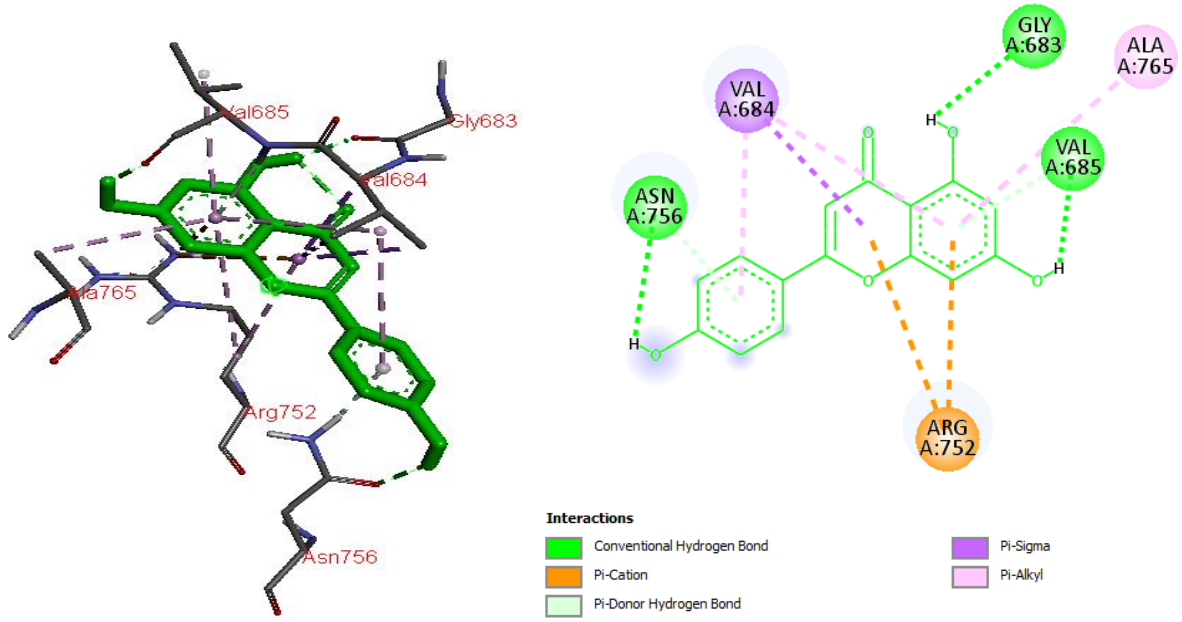

Fig:3 Complex structure of androgen receptor with APIGENIN and amino acid involve in this interaction, name is Asn756, Arg752, Val684, Gly683, Ala765, Val685.

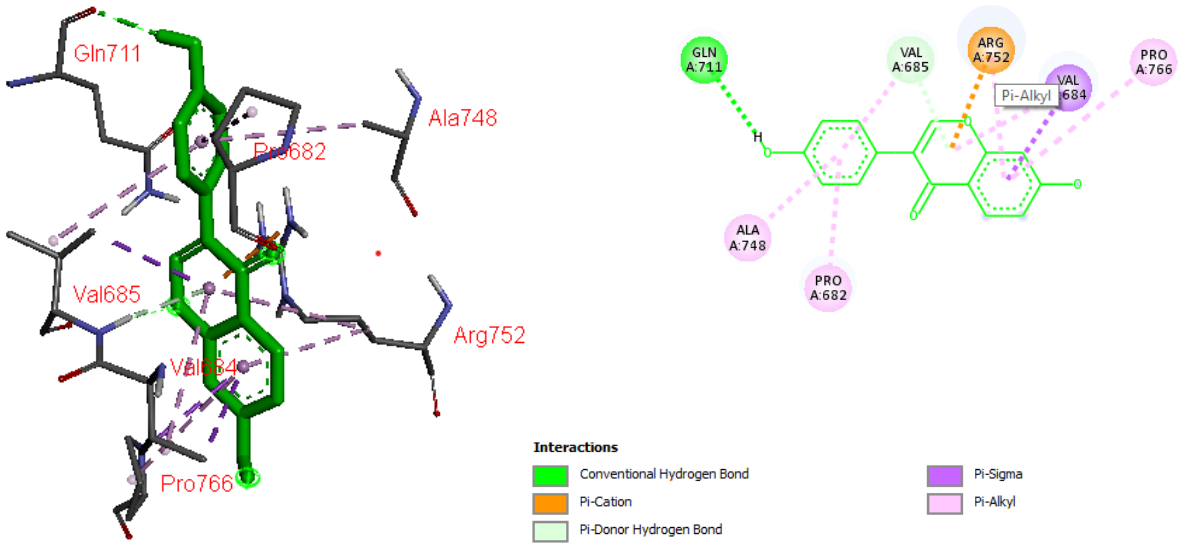

Fig:4 Complex structure of androgen receptor with DAIDZEIN and amino acid involve in this interaction, name is Gln711, Val715, Arg752, Val685, Pro766, Pro682, Ala748.

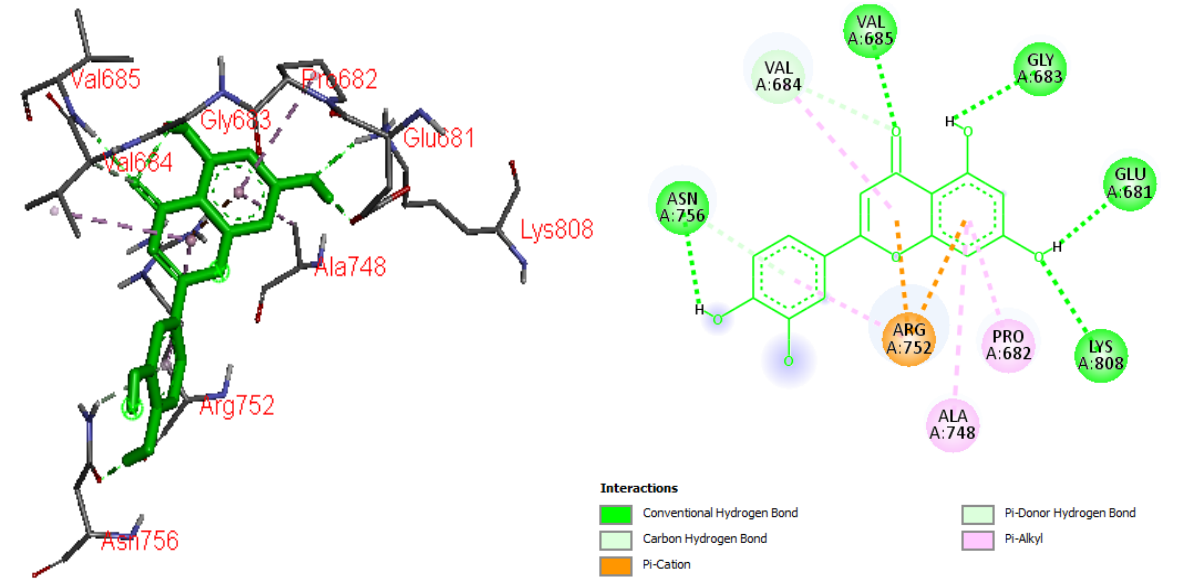

Fig:5 Complex structure formation of androgen receptor with LUTEOLIN and amino acid involves in this interaction, name is Asn756, Val684, Val685, Gly683, Glu681, Lys808, Pro682, Ala748, Arg752.

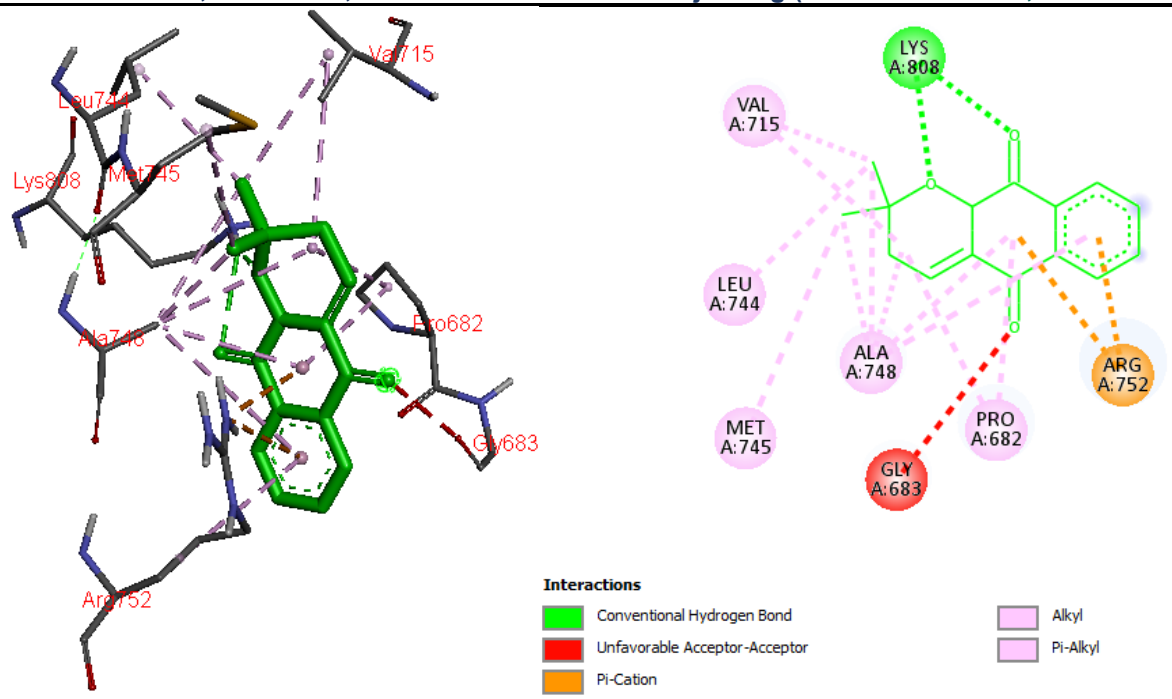

Fig:6 Complex structure formation of androgen receptor with **ALPHA-LAPACHONE** and amino acid involves in this interaction, name is Leu744, Val715, Lys808, Arg752, Pro682, Gly683, Met745, Ala748.

ADME SCREENING

SI NO	NPACT ID	COMPOUND NAME	MOL. FORMULA	MOLWT (g/mol)	SMILE ID
1	NPACT00029	10-Epi-olguine	C18H22O9	382.4	O1[C@@H]([C@@H]1/C=C/[C@@H](OC(=O)C)[C@@H](OC(=O)C)C)[C@@H]1OC(=O)C=C[C@@H]1OC(=O)C
2	NPACT00037	12-Deoxyphorbol 20-acetate 13-angelate	C27H36O7	472.6	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@H]2[C@](O)(CC(=C1)COC(=O)C)C(=O)C(=C2)C)C(=O)/C(=CC)/C
3	NPACT00053	1-beta,6-alpha-dihydroxy-4(15)-eudesmene	C15H26O2	238.37	O[C@@H]1[C@@H]2[C@@](CC[C@H]1C(C)C)([C@H](O)CCC2=C)C
4	NPACT00070	20-hydroxy-12-deoxyphorbol angelate	C25H34O6	430.5	O([C@@]12[C@@H](C1(C)C)[C@H]1[C@](O)([C@@H](C2)C)[C@H]2[C@](O)(CC(=C1)CO)C(=O)C(=C2)C)C(=O)/C(=C/C)/C
5	NPACT00071	20-hydroxyresiniferol 9,13,-14-orthophenylacetate	C28H32O6	464.5	O1[C@@]23[C@H]([C@H]4O[C@]1(O[C@]4(C[C@H]2C)C(=C)CCc1ccccc1)C=C(C[C@@]1(O)[C@H]3C=C(C1=O)C)CO
6	NPACT00089	28-deoxonimbolide	C27H32O6	452.5	O1[C@H]2[C@]([C@@H]([C@@]3([C@H]4[C@H]2OC[C@@]4(C=CC3=O)C)C)CC(=O)OC)(C2=C([C@H](C[C@@H]12)c1ccoc1)C)C
7	NPACT00090	28-homocastasterone	C29H50O5	478.7	OC(CCc1c2c(oc3c(c2=O)c(O)c(c(O)c3)CC=C(C)C)cc(O)c1OC)(C)C
8	NPACT00111	3,6-Epidioxy-1,10-bisaboladiene	C15H24O2	236.35	O1O[C@@]2(CC[C@@]1([C@H](CCC=C(C)C)C)C=C2)C
9	NPACT00111	3'-O-Methyl-6-(1,1-dimethylallyl)eriodictyol	C21H22O6	370.4	O1[C@@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1cc(OC)c(O)cc1

10	NPACT00117	strophanthidin	C23H32O6	404.5	O[C@@]12[C@H]3[C@@H]([C@@]4([C@](O)(CC3)C[C@@H](O)CC4)C=O)CC[C@@]1([C@H](CC2)C1=CC(=O)OC1)C
11	NPACT00129	3'-formyl-2',4',6'-trihydroxy-5'-methyldihydrochalcone	C17H16O5	300.3	Oc1c(C(=O)CCc2ccccc2)c(O)c(c(O)c1C)C=O
12	NPACT00155	4'-demethyldeoxypodophyllotoxin	C21H20O7	384.4	O1C[C@H]2[C@@H]([C@@H](c3c(C2)cc2OCOc2c3)c2cc(OC)c(O)c(OC)c2)C1=O
13	NPACT00156	4'-demethylpodophyllotoxin	C21H20O8	400.4	O1C[C@H]2[C@@H]([C@@H](c3c([C@@H]2O)cc2OCOc2c3)c2cc(OC)c(O)c(OC)c2)C1=O
14	NPACT00165	5,4'-Dihydroxy-4",4"-dimethyl-5"-methyl-5"-H-dihydrofuruno[2",3":6,7]flavonone	C20H20O5	340.4	O1[C@@H](C(c2c1cc1O[C@@H](CC(=O)c1c2O)c1ccc(O)cc1)(C)C)C
15	NPACT00170	5,7-dimethoxy-3',4'-methylenedioxyflavanone	C17H16O4	284.31	O1[C@H](CC(=O)c2c1cc(OC)cc2OC)c1ccccc1
16	NPACT00172	5-desmethylnobiletin	C20H20O9	404.4	o1c2c(c(O)c(OC)c(OC)c2OC)c(=O)c(O)c1c1cc(OC)c(OC)cc1
17	NPACT00173	5-desmethylsinensetin	C39H44N2O8	668.8	o1c2c(c(O)c(OC)c(OC)c2)c(=O)cc1c1cc(OC)c(OC)cc1
18	NPACT00181	6-(1,1-Dimethylallyl)eriodictyol	C20H20O6	356.4	O1[C@@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1cc(O)c(O)cc1
19	NPACT00182	6-(1,1-Dimethylallyl)naringenin	C20H20O5	340.4	O1[C@H](CC(=O)c2c(O)c(C(C)(C)C=C)c(O)cc12)c1ccc(O)cc1
20	NPACT00183	6-(2-Hydroxy-3-methyl-3-butenyl)-8-prenyl-eriodictyol	C25H28O7	440.5	O1[C@@H](CC(=O)c2c1c(c(O)c(c2O)C[C@H](O)C(=C)C)/C=C/C(C)C)c1cc(O)c(O)cc1
21	NPACT00193	6-oxo-pristimerol	NOT FOUND	NOT FOUND	c1c(c(c(c2c1C(C(=CC2=O)C)(C)C)C)O)O
22	NPACT00206	9-alpha-hydroxy-1-beta,10-alpha-epoxyparthenolide	480.6 g/mol	566.6	O1C2(C1C1OC(=O)C(=C)C1CC(O)C1(OC1CC2)C)C
23	NPACT00207	9-alpha-hydroxyparthenolide	$C_{15}H_{20}O_4$	264.32	[C@@H]12CC[C@@]3([C@@H]([C@@H]4[C@H](C[C@@H]([C@@]1(O2)C)O)C(=C)C(=O)O4)O3)C
24	NPACT00208	9-beta-hydroxy-1-beta,10-alpha-epoxyparthenolide	C15H20O5	280.32	O1C2(C1C1OC(=O)C(=C)C1CC(O)C1(OC1CC2)C)C
25	NPACT00270	Apigenin	C15H10O5	270.24	o1c2c(c(=O)cc1c1ccc(O)cc1)c(O)cc(O)c2
26	NPACT00390	Caracasine	C21H30O3	330.5	C(CC(=O)OC)[C@@]1([C@H](C(=C)C)CC[C@]23[C@@H]1CC[C@H](C2)C(=C)C3=O)C
27	NPACT00391	Caracasine acid	C20H28O3	316.4	C(CC(=O)O)[C@@]1([C@H](C(=C)C)CC[C@]23[C@@H]1CC[C@H](C2)C(=C)C3=O)C
28	NPACT00413	Chamaejasmine	C30H22O10	542.5	O1[C@H]([C@H]([C@H]2[C@@H](Oc3c(C2=O)c(O)cc(O)c3)c2ccc(O)cc2)C(=O)c2c1cc(O)cc2O)c1ccc(O)cc1
29	NPACT00476	Daidzein	C15H10O4	254.24	o1c2c(c(=O)c(c3ccc(O)cc3)c1)ccc(O)c2

30	NPACT00495	Deoxypodophyllotoxin	C22H22O7	398.4	
31	NPACT00497	Desmethylxanthohumol	C20H20O5	340.4	Oc1c(CC=C(C)C)c(O)cc(O)c1C(=O)/C=C/c1ccc(O)cc1
32	NPACT00512	Diphyllin	C21H16O7	380.3	O1Cc2c(c(c3c(c2O)cc(OC)c(OC)c3)c2cc3OCOc3cc2)C1=O
33	NPACT00518	Dysosmarol	C20H24O7	376.4	O1[C@H]([C@@H]([C@@H](C1)[C@H](O)c1cc(OC)cc(O)c1)CO)c1cc(OC)c(O)cc1
34	NPACT00565	Escobarine A	C20H26O4	330.4	O1[C@@]2([C@H]3[C@@H]([C@@]4([C@H](C(CCC4)(C)C)C[C@@H]3O)C)CC(=O)[C@]12C#C)C=O
35	NPACT00566	Escobarine B	C20H28O4	332.4	O1[C@@]2([C@H]3[C@@H]([C@@]4([C@H](C(CCC4)(C)C)C[C@@H]3O)C)CC(=O)[C@]12C#C)CO
36	NPACT00665	Honokiol	C18H18O2	266.3	Oc1c(c2cc(c(O)cc2)CC=C)cc(CC=C)cc1
37	NPACT00670	Isobonducellin	C17H14O4	282.29	O1C/C(=C/c2ccc(OC)cc2)/C(=O)c2c1cc(O)cc2
38	NPACT00712	Limocitrin 3,5,7,4'-tetramethyl ether	C21H22O8	402.4	o1c2c(c(=O)c(OC)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2OC
39	NPACT00729	Luteolin	C15H10O6	286.24	o1c2c(c(=O)cc1c1cc(O)c(O)cc1)c(O)cc(O)c2
40	NPACT00817	Nobiletin	C21H22O8	402.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)cc1c1cc(OC)c(OC)cc1
41	NPACT00843	Parthenolid-9-one	NOT FOUND	NOT FOUND	C1=C(C(=O)C[C@@H]2[C@@H]([C@H]3[C@@](CC1)(O3)C)OC(=O)C2)C
42	NPACT00864	Phyllamyricin C	NOT FOUND	NOT FOUND	c1(c(c(cc2c1cc1COC(=O)c1c2c1ccc2c(c1)OCO2)OC)OC)OC
43	NPACT00873	Podophyllotoxone	C22H20O8	412.4	O1C[C@H]2[C@@H]([C@@H](c3c(C2=O)cc2OCOc2c3)c2cc(OC)c(OC)c(OC)c2)C1=O
44	NPACT00888	Purpuracenin	C23H26O10	462.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)c(OC)c1c1c(OC)cc(OC)c(OC)c1
45	NPACT00892	Quercetin 3,5,7,3',4'-pentamethyl ether	C20H20O7	372.4	o1c2c(c(=O)c(OC)c1c1cc(OC)c(OC)cc1)c(OC)cc(OC)c2
46	NPACT00893	Quercetin 3,7,3',4'-tetramethyl ether	C19H18O7	358.3	o1c(c2cc(OC)c(OC)cc2)c(OC)c(=O)c2c1cc(OC)cc2O
47	NPACT00899	Reissantins D	C24H32O8	448.5	O1[C@@]23[C@]([C@@H](OC(=O)c4ccccc4)[C@@H](O)[C@H]([C@H]2O)C1(C)C)([C@@H](OC(=O)C)CC[C@@]3(O)C)C
48	NPACT00965	Syriacusins A	C13H12O4	232.2	O(c1c2c(cc(c1O)C)ccc(O)c2C=O)C
49	NPACT00967	Tangeretin	C20H20O7	372.4	o1c2c(c(OC)c(OC)c(OC)c2OC)c(=O)cc1c1ccc(OC)cc1
50	NPACT00973	Tetra-o-methylisoscutellarein	C18H16O5	312.3	o1c2c(c(OC)cc(OC)c2)c(=O)cc1c1ccc(OC)cc1
51	NPACT00974	Tetra-o-methylscutellarein	C19H18O6	342.3	o1c2c(c(OC)c(OC)c(OC)c2)c(=O)cc1c1ccc(OC)cc1
52	NPACT01012	Wedelolactone	C16H10O7	314.25	o1c2c(c3c1cc(O)c(O)c3)c(=O)oc1c2c(O)cc(OC)c1
53	NPACT01039	(-)-usnic acid	C18H16O7	244.3	O1C2=CC(=C(C(=O)[C@]2(c2c1c(c(O)c(c2O)C)C(=O)C)C)C(=O)C)O

54	NPACT01054	(S)-5-hydroxy-7,4'-dimethoxyflavanone	C17H16O5	300.3	O1C(CC(=O)c2c1cc(OC)cc2O)c1ccc(OC)cc1
55	NPACT01065	2-(1-hydroxyethyl)naphtho[2,3-b]furan-4,9-quinone	C14H10O4	242.2	o1c2c(cc1C(O)C)C(=O)c1c(C2=O)cccc1
56	NPACT01073	2-acetylnaphtho[2,3-b]furan-4,9-quinone	NOT FOUND	NOT FOUND	c1(=C)c2c(c(=C)c3c1[CH][C](O3)C(=O)C)cccc2
57	NPACT01108	9-Aminocamptothecin	C20H17N3O4	363.4	O1Cc2c([C@@](O)(CC)C1=O)cc1n(Cc3c1nc1c(c3)c(N)ccc1)c2=O
58	NPACT01122	alpha-lapachone	C15H14O3	242.2	O1C(CCC2=C1C(=O)c1c(C2=O)cccc1)(C)C
59	NPACT01129	Andrographolide	C20H30O5	350.4	O[C@H]1[C@]([C@@H]2[C@]([C@@H](C(=C)CC2)C/C=C/2[C@H](O)COC2=O)(CC1)C)(CO)C
60	NPACT01187	dehydro-iso-alpha-lapachone	C15H12O3	240.25	O1C(CC2=C1C(=O)c1c(C2=O)cccc1)C(=C)C
61	NPACT01227	Hispidulin	C16H12O6	300.26	o1c2c(c(O)c(OC)c(O)c2)c(=O)cc1c1ccc(O)cc1
62	NPACT01445	(1S,5S,6R,7S,9R,10S)-5-Methylbutanoyloxy-1,4,9-trihydroxy-2-oxoxanth-11-en-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[C@H]1O)C(=C)C(=O)O2)OC(=O)C(C)CC)(O)C(=O)CC(C)O)C
63	NPACT01446	9-Oxo-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(CC1=O)C(=C)C(=O)O2)OC(=O)C(C)CC)(C(=O)/C=C/C)O)C
64	NPACT01453	(1S,5S,6R,7R,8S,10S)-5-Angeloyloxy-1,8-dihydroxy-2-oxoxantha-3,11-dien-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([C@H]([CH]1)O)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
65	NPACT01453	(1S,5S,6R,7R,8S,10S)-5-Angeloyloxy-1,8-dihydroxy-2-oxoxantha-3,11-dien-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([C@H]([CH]1)O)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
66	NPACT01460	(1S,5S,6R,7S,10R)-1-Hydroxy-4-methoxy-5-methylbutanoyloxy-2,9-dioxoxanth-11-en-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[CH]1)C(=C)C(=O)O2)OC(=O)C(CC)C)(O)C(=O)CC(C)OC)C
67	NPACT01467	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-angelate	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([CH][C@H]1O)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C
68	NPACT01479	9-alpha-Hydroxy-seco-ratiferolide-5-alpha-O-(2-methylbutyrate)	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C(C[C@H]1O)C(=C)C(=O)O2)OC(=O)C(C)CC)(O)C(=O)/C=C/C)C
69	NPACT01481	(1S,5S,6R,7S,10S)-5-Angeloyloxy-1-hydroxy-2-oxoxantha-3,11-dien-6,12-olide	NOT FOUND	NOT FOUND	[C@H]1(C([C@H]([C@H]2C([CH][CH]1)C(=C)C(=O)O2)OC(=O)/C(=CC)/C)(C(=O)/C=C/C)O)C

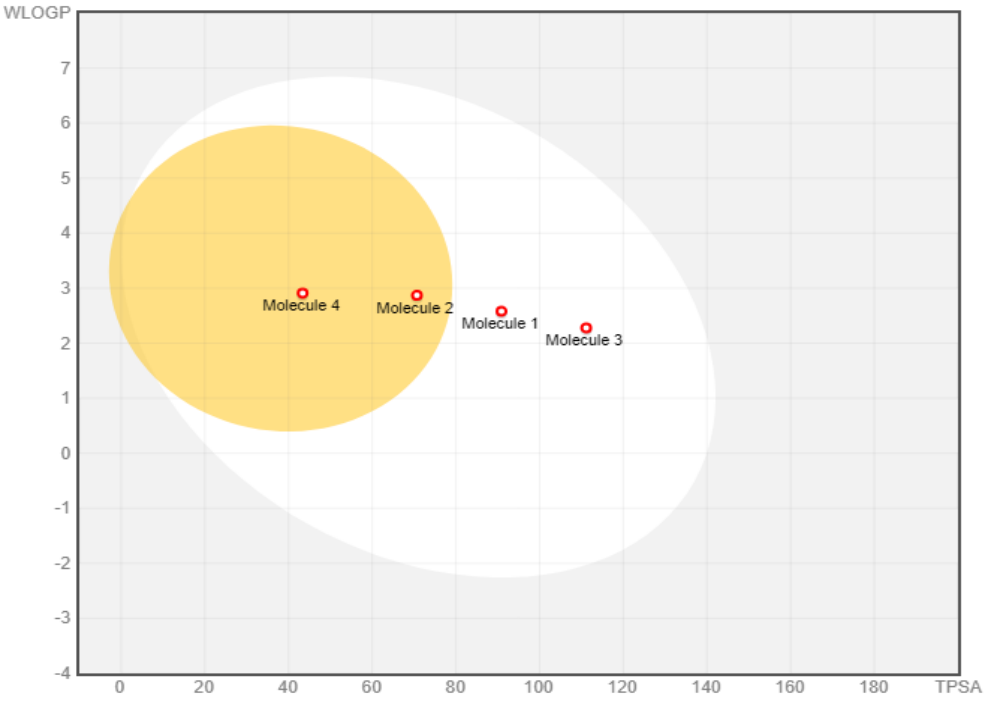

Fig:7 Boiled Egg Score For Best Docked Compounds

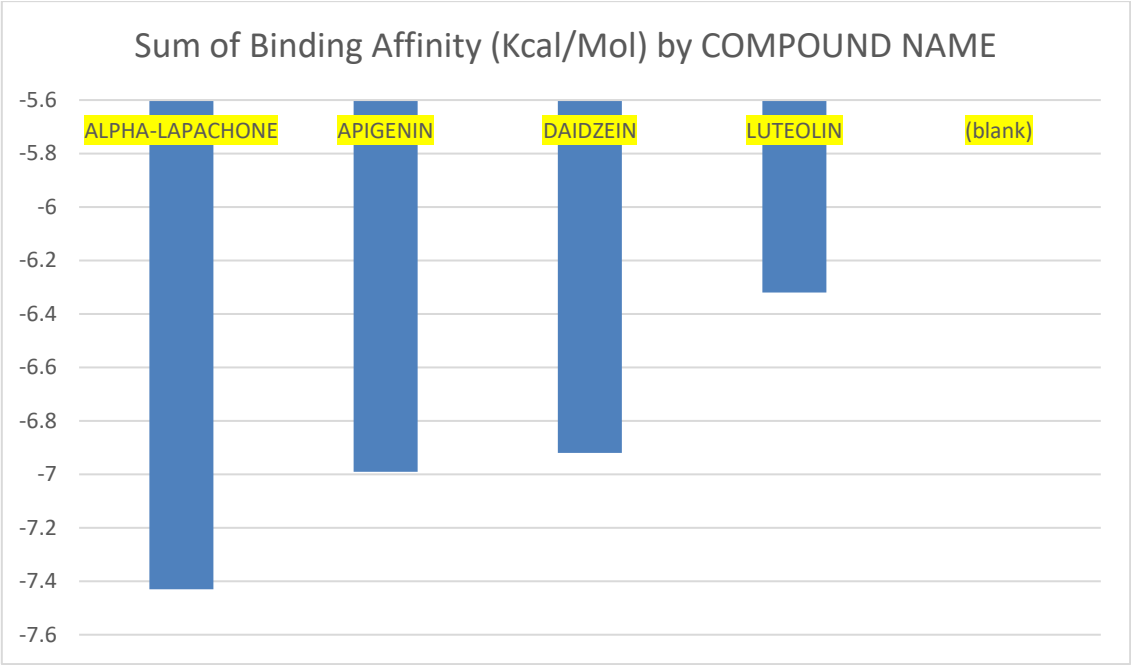

Fig: 8 Figure showing the sum of auto dock binding affinity (kcl/mol) by compound name

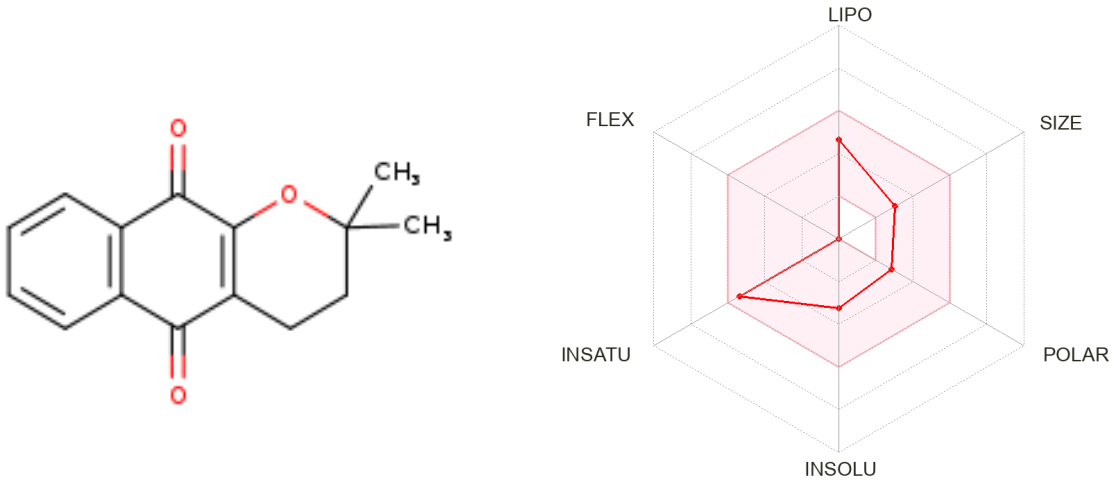

Fig: 9 2D STRUCTURE AND Swiss Radar OF ALPHA-LAPACHONE Potent Inhibitor of Androgen Receptor

7.CONCLUSION AND FEATURE ASPECTS

The ligands with the least binding energy scores were taken. Out of 69 we get 4 molecules with best binding affinity with androgen receptor. (The four molecules are **Apigenin, Daidzein, Luteolin, Alpha-Lapachone)** From these four molecule only one molecule i.e. **Alpha-Lapachone** have best binding affinity in entire docking analyis this molecule is consider as potent inhibitor for androgen receptor. ALPHA-LAPACHONE is found in the barks of catalpa ovata.

After these all study we were go for Phase 2 study on androgen receptor via de novo drug desgining

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