COMPREHENSIVE STUDY OF MARINE – BASED LEAD COMPOUNDS IDENTIFICATION AGAINST GYNECOLOGICAL CANCER TARGETS

Submitted in partial fulfillment of the requirements for the award of Master of Science degree in Bioinformatics and Data Science

By

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INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)
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BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of VAISHNAVI S (40739006) who carried out the project entitled **"COMPREHENSIVE STUDY OF MARINE–BASED LEAD COMPOUNDS IDENTIFICATION AGAINST GYNECOLOGICAL CANCER TARGETS"** under my supervision from to April 2022

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DECLARATION

I **VAISHNAVI S (40739006)** hereby declare that the Project Report entitled **COMPREHENSIVE STUDY OF MARINE BASED LEAD COMPOUNDS IDENTIFICATION AGAINST GYNECOLOGICAL CANCER TARGETS** done by me under the guidance of Dr JEMMY CHRISTY (Internal) and (External) at (Company name and address) is submitted in partial fulfillment of the requirements for the award of Masters of Science degree in Bioinformatics and Data Science.

DATE:

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SIGNATURE OF THE CANDIDATE

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ABSTRACT

Gynecological cancers are among the most common cancers in women and hence an important public health issue. Due to the lack of cancer awareness, variable pathology, and dearth of proper screening facilities in developing countries such as India, most women report at advanced stages, adversely affecting the prognosis and clinical outcomes. Ovarian cancer has emerged as one of the most common malignancies affecting women in India and has shown an increase in the incidence rates over the years. Cancer has become an important public health problem with over 800,000 new cases occurring every year in India. It is estimated that there are nearly 2.5 million cases in the country with nearly 400,000 deaths occurring due to cancer. Many marine-derived natural products and their analogues have been reported to show antiangiogenic activities. Compared with the drugs in the clinic, these agents display interesting characteristics, including diverse sources, unique chemical structures, special modes of action, and distinct activity and toxicity profiles. Cancer remains one of the most lethal diseases worldwide. There is an urgent need for new drugs with novel modes of action and thus considerable research has been conducted for new anticancer drugs from natural sources, especially plants, microbes and marine organisms. Marine populations represent reservoirs of novel bioactive metabolites with diverse groups of chemical structures. The impact of marine organisms, with particular emphasis on marine plants, bacteria, fungi, sponges' Anti-cancer effects of marine natural products in in vitro and in vivo studies were first introduced; their activity in the prevention of tumor formation and the related compound-induced apoptosis and cytotoxicity were tackled.

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CHAPTER 1 - INTRODUCTION

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LIST OF ABBREVIATIONS

HPV - human papillomavirus vaccine

FDA - Food and Drug Administration

PIK3CA - phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit alpha.

PCR - polymerase chain reaction

CMNPD **-** Comprehensive Marine Natural Products Database

PTEN - Phosphatase and tensin homolog

TOPKAT - Toxicity Prediction by Komputer Assisted Technology

HOMO - highest occupied molecular orbital

LUMO -lowest unoccupied molecular orbital

PDB - Protein Data Bank

RMSF – Root mean square fluctuation

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INTRODUCTION

CANCER

Cancer is a disease caused when cells divide uncontrollably and spread into surrounding tissues. Cancer is caused by changes to DNA. Most cancer-causing DNA changes occur in sections of DNA called genes. These changes are also called genetic changes. Cancer can start almost anywhere in the human body, which is made up of trillions of cells. Cancer is a disease in which some of the body's cells grow uncontrollably and spread to other parts of the body. Cancer can start almost anywhere in the human body, which is made up of trillions of cells. Normally, human cells grow and multiply (through a process called cell division) to form new cells as the body needs them. When cells grow old or become damaged, they die, and new cells take their place. Cancer is a genetic disease that is caused by changes to genes that control the way our cell's function, especially how they grow and divide. A cancer that has spread from the place where it first formed to another place in the body is called metastatic cancer. Fearon ER The process by which cancer cells spread to other parts of the body is called metastasis. There are more than 100 types of cancer. Types of cancer are usually named for the organs or tissues where the cancers form. For example, lung cancer starts in the lung, and brain cancer starts in the brain. Cancers also may be described by the type of cell that formed them, such as an epithelial cell or a squamous cell. Sometimes this orderly process breaks down, and abnormal or damaged cells grow and multiply when they shouldn't. These cells may form tumors, which are lumps of tissue. Tumors can be cancerous or not cancerous(benign).

CANCER PREVALENCE WORLDWIDE

Cancer ranks as a leading cause of death and an important barrier to increasing life expectancy in every country of the world.1 According to estimates from the World Health Organization (WHO) in 2019, 2 cancer is the first or second leading cause of death before the age of 70 years in 112 of 183 countries and ranks third or fourth in a further 23 countries. Cancer's rising prominence as a leading cause of death partly reflects marked declines in mortality rates of stroke and coronary heart disease, relative to cancer, in many countries. Overall, the burden of cancer incidence and mortality is rapidly growing worldwide; this reflects both aging and growth of the population as well as changes in the

prevalence and distribution of the main risk factors for cancer, several of which are associated with socioeconomic development.

CANCER INCIDENCE AND DEATH RATES BY SEX AND WORLD REGION

Worldwide, the incidence rate for all cancers combined was 19% higher in men (222.0 per 100,000) than in women (186 per 100,000) in 2020, although rates varied widely across regions. Among men, incidence rates ranged almost 5-fold, from 494.2 per 100,000 in Australia/New Zealand to 100.6 per 100,000 in Western Africa; among women, rates varied nearly 4-fold, from 405.2 per 100,000 in Australia/New Zealand to 102.5 per 100,000 in South Central Asia. These variations largely reflect differences in exposure to risk factors and associated cancers (cancer mix) and barriers to high-quality cancer prevention and early detection. The gender gap for overall cancer mortality worldwide is twice that for incidence, with death rates 43% higher in men than in women (120.8 and 84.2 per 100,000, respectively), partly because of differences in the distribution of the cancer types. Death rates per 100,000 persons varied from 165.6 per 100,000 in Eastern Europe to 70.2 per 100,000 in Central America among men and from 118.3 per 100,000 in Melanesia to 63.1 per 100,000 in Central America and South-Central Asia among women. Notably, the cumulative risk of dying from cancer among women in 2020 was higher in Eastern Africa (11.0%) than in Northern America (8.2%), Western Europe (8.8%), and Australia/New Zealand (7.4%). Europe accounts for 22.8% of the total cancer cases and 19.6% of the cancer deaths, although it represents 9.7% of the global population, followed by the Americas' 20.9% of incidence and 14.2% of mortality worldwide. In contrast to other regions, the share of cancer deaths in Asia (58.3%) and Africa (7.2%) are higher than the share of incidence (49.3% and 5.7%, respectively) because of the different distribution of cancer types and higher case fatality rates in these regions **(Freddie Bray et al., 2018)**

GYNECOLOGICAL CANCERS:

Gynecologic cancer is any cancer that starts in a woman's reproductive organs. Five main types of cancer affect a woman's reproductive organs are cervical, ovarian, uterine,

vaginal and vulvar. As a group, they are referred to as gynecologic cancer. A sixth type of gynecologic cancer is the very rare fallopian tube cancer. The five gynecologic cancers begin in different places within a woman's pelvis, which is the area below the stomach and in between the hip bones. Each gynecologic cancer is unique, with different signs and symptoms, different risk factors and different prevention strategies. All women are at risk for gynecologic cancers, and risk increases with age. When gynecologic cancers are found early, treatment is most effective**. (Maheshwari A et.al 2018)**

COMMON SYMPTOMS OF GYNECOLOGIC CANCERS*:*

Abnormal vaginal bleeding or discharge is common in all gynecologic cancers except vulvar cancer. Feeling full too quickly or difficulty eating, bloating, and abdominal or back pain are common only for ovarian cancer. Pelvic pain or pressure is common for ovarian and uterine cancers. More frequent or urgent need to urinate and/or constipation are common for ovarian and vaginal cancers. Itching, burning, pain, or tenderness of the vulva, and changes in vulva color or skin, such as a rash, sores, or warts, are found only in vulvar cancer. **(Beharee N et al., 2019).**

PREVENTION

HPV vaccination is recommended for preteens aged 11 to 12 years, but can be given starting at age 9.HPV vaccine also is recommended for everyone through age 26 years, if they are not vaccinated already HPV vaccination is not recommended for everyone older than age 26 years. However, some adults' age 27 through 45 years who are not already vaccinated may decide to get the HPV vaccine after speaking with their doctor about their risk for new HPV infections and the possible benefits of vaccination. HPV vaccination in this age range provides less benefit, as more people have already been exposed to HPV. If vaccination is started before age 15, a two-dose schedule is recommended, with the doses given 6 to 12 months apart. For people who start the series after their 15th birthday, the vaccine is given in a series of three shots**. (Karthikeyan K. 2018)**

TYPES OF GYNECOLOGICAL CANCERS:

- Uterine cancer
- Cervical cancer
- Ovarian cancer
- Vulvar cancer
- Vaginal cancer

i.*Uterine cancer:*

Uterine cancer is cancer that begins in the uterus and is one of the most common types of gynecological cancers. Though it can happen to anyone, some factors which increase the risk of **uterine cancer** are obesity, diabetes, hypertension, use of estrogen without progesterone, etc. **(Uma Devi K 2017)**

ii.*Cervical cancer:*

Another very common type of gynecologic cancer is **cervical cancer** and is one of the leading causes of cancer-related deaths in women worldwide. A large number of women in India are diagnosed with this cancer every year, and unfortunately, due to lack of awareness and poor **cancer screening** facilities, a majority of women are diagnosed when cancer has reached advanced stages. Also, a large number of cervical cancers are caused due to HPV (Human Papillomavirus) infection. **(Uma Devi K 2017)**

iii.*Ovarian cancer:*

Ovarian cancer is another common gynecological cancer. There are three types of it: epithelial ovarian cancer, germ cell cancer, and stromal cell cancer. Of these, epithelial ovarian cancer is the most common one accounting for about 85 percent of all ovarian cancers. **(Uma Devi K 2017)**

iv.*Vulvar cancer:*

Vulvar cancer is a rare form of gynecological cancer and it affects the external female genitalia. Vulvar cancer is a highly curable type of gynecological cancer. In most cases,

radical surgery is sufficient to treat vulvar cancer but some cases may require chemotherapy and radiation therapy as well. **(Uma Devi K 2017)**

v.*Vaginal cancer:*

Cancer that forms in the tissues of the vagina (birth canal). The vagina leads from the cervix (the opening of the uterus) to the outside of the body. The most common type of vaginal cancer is squamous cell carcinoma, which starts in the thin, flat cells lining the vagina. Another type of vaginal cancer is adenocarcinoma, cancer that begins in glandular cells in the lining of the vagina**. (Uma Devi K 2017)**

GYNECOLOGICAL CANCER STATISTICS IN WORLDWIDE

The International Agency for Research on Cancer has estimated that gynecologic cancers accounted for 19% of the more than 5 million new cancer cases and nearly 3 million deaths among women worldwide, an estimated 14,100 women in the United States will be diagnosed with invasive cervical cancer. Worldwide, an estimated 604,127 women were diagnosed with cervical cancer in 2020**. (Thompson CA et al.,2016)** Compared to other types of cancer (like breast or colon cancer), gynecologic cancers are uncommon, occurring in about 100,000 women in the United States each year. That said, all women are at risk for developing gynecologic cancers, and the risk increases with age. Cervical cancer is the fourth most commonly occurring cancer in women and the eighth most commonly occurring cancer overall. There were over 500,000 new cases in 2018.

GYNECOLOGICAL CANCER STATISTICS IN INDIA

Every year in India, 122,844 women are diagnosed with cervical cancer and 67,477 die from this disease. Over the past years, many Indian researchers have published studies in gynecologic oncology, and this review discusses the important work done in this field. Ovarian and cervical cancers are the most common gynecological cancers affecting women worldwide and in India. Every four minutes, Indian women are diagnosed with breast cancer **(Maheshwari A et al.,2018)** In India, cervical cancer contributes to approximately 6–29% of all cancers in women. The age-adjusted incidence rate of

cervical cancer varies widely among registries; highest is 23.07/100,000 in Mizoram state and the lowest is 4.91/100,000 in Dibrugarh district. **(Amita et al 2019)**

GYNECOLOGIC CANCER TREATMENT OPTIONS

Robotic-Assisted Gynecological Cancer Surgery Magee also offers robotic-assisted surgery for some gynecologic procedures, such as:

- Hysterectomies
- Removal of cancerous tumors
- Removal of both fallopian tubes and ovaries (bilateral salpingo-oophorectomy) **(Clair KH, et.al 2020)**

CHEMOTHERAPY AND HORMONE THERAPY

Some gynecologic cancers can be treated with chemotherapy alone. Others may require surgical removal prior to chemotherapy treatment and potentially radiation therapy to prevent local recurrence. Depending on the type and stage of the cancer, chemotherapy may be:

- Taken by mouth
- Given as an injection
- Placed directly into the tumor site **(Kiran H et al., 2020)**

WHY NATURAL MARINE COMPOUND

Marine natural products can be defined as biologically active products as secondary metabolites as well as enzymes, lipids, and heteropolysaccharides. From: Synthesis of Medicinal Agents from Plants. In total, over 30,000 marine natural products have been discovered since the first report of biologically active spongothymidine in 1950. As of writing, several marine-derived drugs have since been approved by the FDA, including Ziconotide and Eribulin, and there are many more candidates in clinical trials**(Atanas G. Atanaso et. Al 2021).** Numerous ecological studies have shown that secondary metabolites produced by sponges often serve defensive purposes to protect them from

threats such as predator attacks, microbial infections, biofouling, and overgrowth by other sessile organisms. Fungi isolated from the deep-sea samples are one of the most pivotal and promising sources for bioactive compounds, presumably owing to the chemical diversity and biodiversity of their secondary metabolites that could be used for drug discovery and pharmacological applications. Bacterial natural products are secondary metabolites formed by biosynthetic enzymes encoded within the bacterial genome.

WHY PIK3CA AS A DRUG TARGET

PIK3CA somatic mutations would be ideal for targeting due to their high rate of occurrence and the fact that 80% to 90% of these mutations are in one of three recurrent hotspot sequences. The development of targeted therapies with true specificity for cancer relies upon exploiting differences between cancerous and normal cells. Genetic and genomic alterations including somatic mutations, translocations, and amplifications have served as recent examples of how such differences can be exploited as effective drug targets. Small molecule inhibitors and monoclonal antibodies directed against the protein products of these genetic anomalies have led to cancer therapies with high specificity and relatively low toxicity**. (Cosgrove DPet al., 2008)** Recently, our group and others have demonstrated that somatic mutations in the PIK3CA gene occur at high frequency in breast and other cancers. Moreover, the majority of mutations occur at three hotspots, making these ideal targets for therapeutic development. Here we review the literature on PIK3CA mutations in cancer, as well as existing data on PIK3CA inhibitors and inhibitors of downstream effectors for potential use as targeted cancer therapeutics**.(Gustin, John P.et.al., 2018)**Prior to the discovery of somatic PIK3CA mutations in human cancers, the PI3K enzyme was already recognized as being an important molecule in mediating carcinogenesis. The phosphatidylinositol 3-kinase (PI3K) p110α catalytic subunit, *PIK3CA*, is one the most highly mutated oncogenes in human cancers, and high mutational frequencies of *PIK3CA* have been reported in colorectal, breast and liver cancers while lower rates of mutation have been described in many other human malignancies including ovarian, lung, gastric, and brain cancers **(Fusco N et al,.2021).**

LITERATURE SURVEY

GYNECOLOGICAL CANCER

Gynecologic oncology is a specialized field of medicine that focuses on cancers of the female reproductive system, including ovarian cancer, uterine cancer, vaginal cancer, cervical cancer, and vulvar cancer. Gynecologic cancer is any cancer that starts in a woman's reproductive organs. Five main types of cancer affect a woman's reproductive organs are cervical, ovarian, uterine, vaginal and vulvar. As a group, they are referred to as gynecologic cancer. A sixth type of gynecologic cancer is the very rare fallopian tube cancer. The five gynecological cancers begin in different places within a woman's pelvis, which is the area below the stomach and in between the hip bones. **(Maheshwari A et al.,2018)** Each gynecologic cancer is unique, with different signs and symptoms, different risk factors and different prevention strategies. All women are at risk for gynecological cancers, and risk increases with age. When gynecological cancers are found early, treatment is most effective. Of all the gynecologic cancers, only cervical cancer has screening tests that can find this cancer early, when treatment can be most effective. Gynecological cancers comprise 10-15% of women's cancers, mainly affecting women past reproductive age but posing threats to fertility for younger patients. The most common route for treatment is combination therapy, consisting of a mix of both surgical and non-surgical interventions (radiotherapy, chemotherapy). **(Amita et al.,2019).**

FDA APPROVED DRUGS OF MARINE ORIGIN

Some of the drugs of marine origin approved for human use in different parts of the world are as follows:

Cytarabine is a synthetic pyrimidine nucleoside derived from spongothymidine and primarily isolated from a Caribbean sponge species Tethya crypta. It is FDA approved and mainly used in different types of leukemia, including acute myelocytic leukemia, lymphocytic leukemia, meningeal leukemia, and blast crisis phase of chronic myelogenous leukemia.

Vidarabine is a synthetic purine nucleoside isolated from the Caribbean sponge T. crypta and developed from spongouridine is currently obtained from Streptomyces antibiotics. It is approved by FDA for use in recurrent epithelial keratitis caused by HSV) type 1 and 2, acute kerato-conjunctivitis, and also for superficial keratitis.

Ziconotide is a synthetic molecule, equivalent to a natural 25-amino acid peptide, v-conotoxin MVIIA. It is originally extracted and purified from the venom of marine snail C. magus, which is a fish-hunting species. Ziconotide has shown potential as an analgesic with a novel mechanism of action. It is approved as an analgesic by the FDA.

A marine natural product extracted from a tunicate species Ecteinascidia turbinata generally inhabitant of Mediterranean and Caribbean Sea. Trabectedin molecule is an alkaloid of tetrahydroisoquinoline class, and it was the first anticancer molecule of marine origin got approval in EU for use in the treatment of soft-tissue sarcoma and in relapsed cases of platinum-sensitive ovarian cancer**. (Malve H 2016).**

MARINE SPONGES

Sponges have been around for a very long time, with certain species having a fossil record that dates back approximately 600 million years to the earliest (Precambrian) period of Earth's history. Marine sponges are sessile invertebrates that can be found in temperate, polar and tropical regions. They are known to be major contributors of bioactive compounds, which are discovered in and extracted from the marine environment**. (Mostafa O et al., 2021).** The compounds extracted from these sponges are known to exhibit various bioactivities, such as antimicrobial, antitumor and general cytotoxicity; simple aquatic animals with dense, yet porous, skeletons are highly adapted to their environments. Sponges are very simple creatures with no tissues. Sponges produce a different kind of chemical substance with numerous carbon skeletons, which have been found to be the main component interfering with human pathogenesis at different sites. The fact that different diseases have the capability to fight at different sites inside the body can increase the chances to produce targeted medicines**(Wei J, et.at., 2020)**

MARINE FUNGI

Marine fungi are species of fungi that live in marine or estuarine environments. They are not a taxonomic group, but share a common habitat **(Gladfelter AS et at 2019).** Obligate marine fungi grow exclusively in the marine habitat while wholly or sporadically submerged in sea water. Facultative marine fungi normally occupy terrestrial or freshwater habitats, but are capable of living or even sporulating in a marine habitat. About 444 species of marine fungi have been described, including seven genera and ten species of basidiomycetes, and 177 genera and 360 species of ascomycetes**. (Wei J et at., 2020)** The remainder of the marine fungi are chytrids and mitosporic or asexual fungi. Many species of marine fungi are known only from spores and it is likely a large number of species have yet to be discovered. Fungi play a dominant role in terrestrial environments where they thrive in symbiotic associations with plants and animals and are integral to nutrient cycling in diverse ecosystems. Marine fungi can be saprobic or parasitic on animals, saprobic or parasitic on algae, saprobic on plants or saprobic on dead wood**(Wiese J et al.,2019).**

MARINE BACTERIA

Bacteria in the ocean adapt to be best suited for their environment. Microbes are everywhere, including the ocean. A single liter of seawater has about one billion bacteria and 10 billion viruses. Marine microorganisms are defined by their habitat as microorganisms living in a marine environment, that is, in the saltwater of a sea or ocean or the brackish water of a coastal estuary. **(Stincone P et.al.,2019)** Those that are close to the water's surface, like cyanobacteria, tend to be photosynthesized. Bacteria constitute a large domain of prokaryotic microorganisms. Typically, a few micrometers in length, bacteria have a number of shapes, ranging from spheres to rods and spirals. **(Wei J et.al., 2020)** Bacteria were among the first life forms to appear on Earth, and are present in most of its habitats. Bacteria inhabit soil, water, acidic hot springs, radioactive waste–and the deep portions of Earth's crust Bacteria also live in symbiotic and parasitic relationships with plants and animals**. (Wiese J et at., 2018)**

PIK3CA (**phosphatidylinositol-4, 5-bisphosphate 3-kinase catalytic subunit alpha)**

PIK3CA (Phosphatidylinositol-4,5-Bisphosphate 3-Kinase Catalytic Subunit Alpha) is a Protein Coding gene. Diseases associated with PIK3CA include Hepatocellular Carcinoma and Megalencephaly- Capillary Malformation-Polymicrogyria Syndrome. PIP3 plays a key role by recruiting PH domain-containing proteins to the membrane, including AKT1 and PDPK1, activating signaling cascades involved in cell growth, survival, proliferation, motility and morphology. Participates in cellular signaling in response to various growth factors. Involved in the activation of AKT1 upon stimulation by receptor tyrosine kinases ligands such as EGF, insulin, IGF1, VEGF and PDGF (**John E Burke et.al., 2018**). Involved in signaling via insulin-receptor substrate (IRS) proteins. Essential in endothelial cell migration during vascular development through VEGFA signaling, possibly by regulating RhoA activity. Required for lymphatic vasculature development, possibly by binding to RAS and by activation by EGF and FGF2, but not by PDGF. Regulates invadopodia formation through the PDPK1-AKT1 pathway. Participates in cardiomyogenesis in embryonic stem cells through an AKT1 pathway. Participates in vasculogenesis in embryonic stem cells through PDK1 and protein kinase C pathway. In addition to its lipid kinase activity, it displays a serine-protein kinase activity that results in the autophosphorylation of the p85alpha regulatory subunit as well as phosphorylation of other proteins such as 4EBP1, H-Ras, the IL-3 beta c receptor and possibly others (**Samantha DiGrande 2019).**

PIK3CA FDA APPROVED INHIBITORS

FDA approved alpelisib (Piqray), an oral drug to be used in combination with endocrine therapy fulvestrant for the treatment of men and postmenopausal women with hormone receptor (HR-positive), human epidermal growth factor receptor 2 (HER2)-negative, PIK3CA-mutated, advanced or metastatic breast cancer following disease progression on or after an endocrine-based regimen) .Common adverse events seen with alpelisib are high blood sugar, increase in creatinine, diarrhea, rash, decrease in lymphocyte count, elevated liver enzymes, nausea, fatigue, low red blood cell count, vomiting, and weight loss, among others. The drug approval also comes with the approval for its companion diagnostic test, therascreen PIK_3CA RGQ PCR Kit, to detect the PIK_3CA mutation in a tissue and/or liquid biopsy. However, as noted by the FDA, patients who are negative by the therascreen test using the liquid biopsy should undergo a tumor biopsy to test for the PIK_3CA mutation. Piqray is the first PI3K inhibitor to demonstrate a clinically meaningful benefit in treating patients with this type of breast cancer **(Samantha Di Grande** 2019) .

AIM AND SCOPE

Gynecological Oncology, is the primary educational and informational publication for topics relevant to detection, prevention, diagnosis, and treatment of gynecologic malignancies. Gynecologic Oncology clinical and investigative articles that concern tumors of the female reproductive tract. Investigations relating to the etiology, diagnosis, and treatment of female cancers.

MATERIALS AND METHODS

CMNPD (*Comprehensive Marine Natural Products Database*)

CMNPD, a comprehensive marine natural products database based on manually curated data, CMNPD currently contains more than 31 000 chemical entities with various physicochemical and pharmacokinetic properties, standardized biological activity data, systematic taxonomy and geographical distribution of source organisms, CMNPD contains 31 561 distinct chemical entities of MNPs from over 13 000 sampling organisms. These organisms are distributed in 7 kingdoms, 38 phyla, 93 classes, 289 orders, 682 families, 1480 genera and 3354 species. There are 15 774 active compounds mapped to 2652 targets with 72 343 bioactivities. These targets include 1122 single proteins, 923 cell lines, 459 organisms and several other types. The document library includes 128 488 scientific literature and patents, of which ∼11 000 articles describe the discovery of new compounds and structure revisions**. (Lyu C, et.at.,2021).**

PIK3CA

PIK3CA (Phosphatidylinositol-4,5-Bisphosphate 3-Kinase Catalytic Subunit Alpha) is a Protein Coding gene. Diseases associated with PIK3CA include Hepatocellular Carcinoma and Megalencephaly -Capillary Malformation- Polymicrogyria Syndrome. A highly significant association between PIK3CA mutations and retention of PTEN protein expression was observed. In addition, PIK3CA mutations were associated with expression of estrogen and progesterone receptors (ER/PR), lymph node metastasis, and ERBB2 overexpression. The fact that PIK3CA mutations and PTEN loss are nearly mutually exclusive implies that deregulated phosphatidylinositol-3,4,5-triphosphate (PIP(3)) is critical for Tumorigenesis in a significant fraction of breast cancers and that loss of PIP(3) homeostasis by abrogation of either PIK3CA or PTEN relieves selective

pressure for targeting of the other gene. The correlation of PIK3CA mutation to ER/PR-positive tumors and PTEN loss to ER/PR-negative tumors argues for disparate branches of tumor evolution. Furthermore, the association between ERBB2 overexpression and PIK3CA mutation implies that more than one input activating the PI3K/AKT pathway may be required to overcome intact PTEN**. (Gillian Leigh Dornan et.al.,2018).**

SwissADME

A free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. SwissADME web tool that gives free access to a pool of fast yet robust predictive models for physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry friendliness, among which in-house proficient methods such as the BOILED-Egg, iLOGP and Bioavailability Radar. Easy efficient input and interpretation are ensured thanks wto a user-friendly interface through the login-free website http://www.swissadme.ch. **(Diana A, et.al.,2017)**

PHARMACOKINETICS

Pharmacokinetics is currently defined as the study of the time course of drug absorption, distribution, metabolism, and excretion. Clinical pharmacokinetics is the application of pharmacokinetic principles to the safe and effective therapeutic management of drugs in an individual patient. **(Shikov AN et.al., 2020).**

TOPKAT

Top Kat (Toxicity Prediction by Komputer Assisted Technology) is a BIOVIA software, a brand of Dassault Systems. The TOPKAT computer-based system for predicting chemical carcinogens was evaluated by determining its ability to predict the carcinogenicity of chemicals tested by the National Toxicology Program. TOPKAT was not effective in identifying potential rodent carcinogens and anticarcinogens in the data set analyzed**. (Prival MJ et al., 2017).**

PHARMACOPHORE

Pharmacophore-based techniques currently are an integral part of many computer-aided drug design workflows and have been successfully and extensively applied for tasks such as virtual screening, de novo design, and lead optimization. Pharmacophore models can be derived both in a receptor-based and in a ligand-based manner, and provide an abstract description of essential non-bonded interactions that typically occur between small-molecule ligands and macromolecular targets. Due to their simplistic and abstract nature, pharmacophores are both perfectly suited for efficient computer processing and easy to comprehend by life and physical scientists**. (Seidel T et.al., 2019)**

MOLECULAR DOCKING

Molecular docking is a key tool in structural molecular biology and computer-assisted drug design. The goal of ligand-protein docking is to predict the predominant binding mode(s) of a ligand with a protein of known three-dimensional structure. Successful docking methods search high-dimensional spaces effectively and use a scoring function that correctly ranks candidate dockings. Docking can be used to perform virtual screening on large libraries of compounds, rank the results, and propose structural hypotheses of how the ligands inhibit the target, which is invaluable in lead optimization. **(Morris GM et al.,2008)**

MOLECULAR ORBITAL

HOMO stands for ‘Highest Occupied Molecular Orbital’, and LUMO stands for ‘Lowest Unoccupied Molecular Orbital’. The HOMO is the highest energy MO that has any electrons in it. The LUMO is the next highest energy orbital {it will be empty}. (Li H et. al., 2018). The LUMO is the lowest energy place to put or excite an electron. The energy difference between the HOMO and LUMO or HOMO-LUMO gap is generally the lowest energy electronic excitation that is possible in a molecule. The energy of the HOMO-LUMO gap can tell us about what wavelengths the compound can absorb. The greater the mobility of the π electrons in large conjugated π orbital systems, the greater the

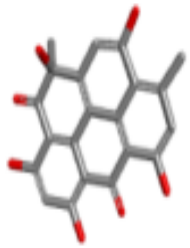
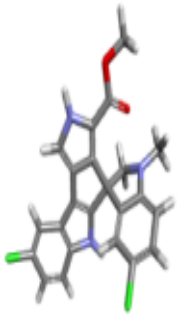
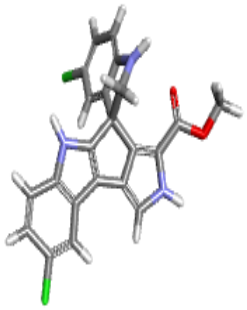
distribution of the energy throughout the molecule, stabilizing it. Hence, smaller HOMO-LUMO gaps correspond to better stability**. (Al-Saadon R et.al., 2018).**

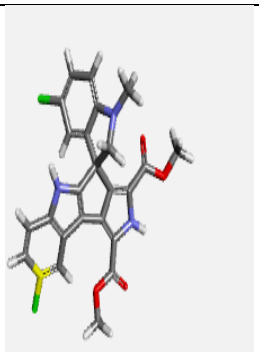
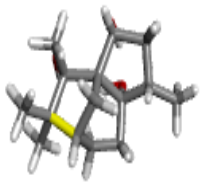
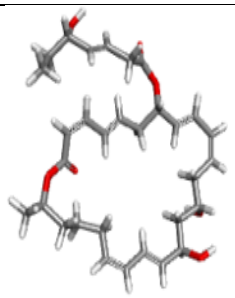
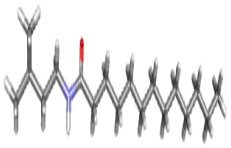
RMSF CABS FLEX

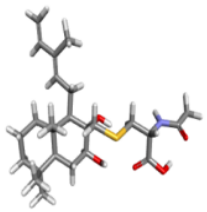
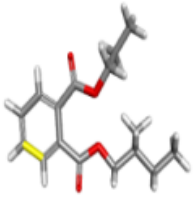
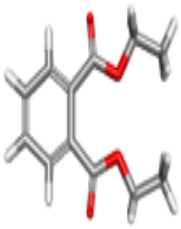
CABS-flex is an efficient modeling procedure for fast simulations of protein structure flexibility. (Kuriata, A. et al.,2018) CABS-flex methodology is a component of the CABS-dock method for protein-peptide docking, which allows for significant flexibility of the peptide and the protein receptor during explicit simulation of peptide binding. (Ciemny, M.P et.al., 2016) The only data required as input is a protein structure in the PDB format (or a protein PDB code). The input structure is used as a starting point for the CABS simulation. The resulting trajectory is automatically analyzed and processed to provide a useful description of protein dynamics. **(Webb, B 2017).**

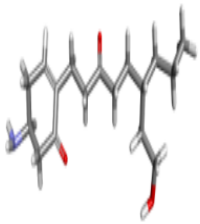
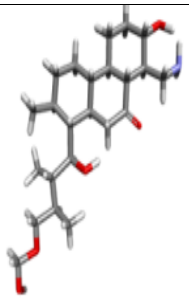
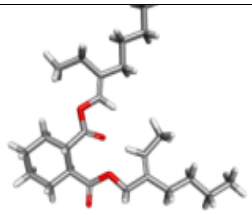
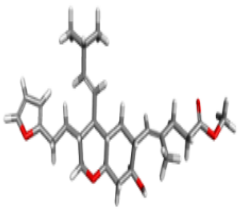
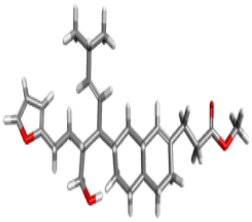
RESULTS AND DISCUSSION

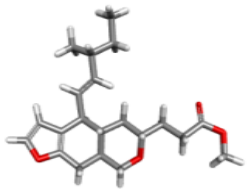
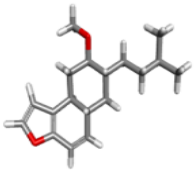
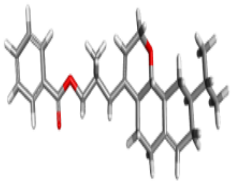
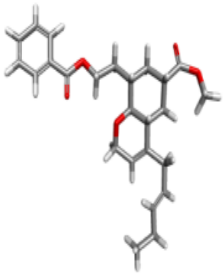
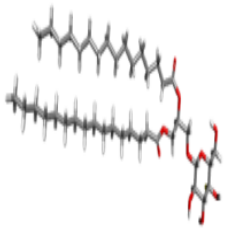
TABLE 5.1 COMPOUND DETAILS FOR MARINE BACTERIA

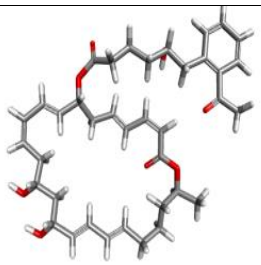
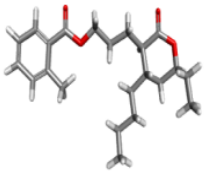
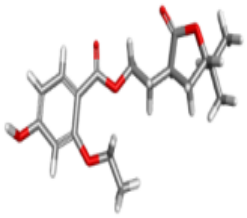
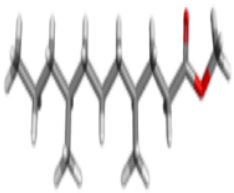
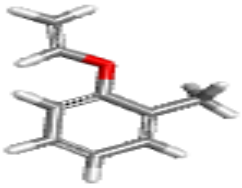
COMPOUND IDENTIFIER	COMPOUND NAME	STRUCTURE	REFERENCE
CMNPD14698	2,4,7,10,14-pentahydroxy-7,12-dimethylpentan cyclo[13.3.1.05,18.08,17.011,16]nonadeca-1,3,5(18),8(17),9,11,13,15-octaene-6,19-dione		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD21959	dimethyl (7S)-5',9-dichlorospiro[4,13-diazatetracyclo[6.6.1.02,6.012,15]pentadeca-1(14),2,5,8(15),9,11-hexaene-7,3'-indole]-3,5-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2015;32(2):116-211. doi:1 doi:10.1039/c5np00156k 0.1039/c4np00144c
CMNPD21961	methyl (3R)-4',5-dichlorospiro[1,2-dihydroindole-3,10'-8,13-diazatetracyclo[7.6.0.02,7.011,15]pentadeca-1(9),2(7),3,5,11,14-hexaene]-12'-carboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k 0.1039/c4np00144c

CMNPD21962	dimethyl (3R)-4',5-dichloro-1-methylspiro[2H-indole-3,10'-8,13-diazatetracyclo[7.6.0.02,7.011,15]pentadeca-1(9),2(7),3,5,11,14-hexaene]-12',14'-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2015;32(2):116-211. doi:10.1039/c4np00144c
CMNPD23280	(1R,2R,4S,5S,8S,10S)-4,9,9,10-tetramethyltricyclo[6.2.1.01,5]undecane-2,5,10-triol		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2012;29(2):144-222. doi:10.1039/c2np00090c
CMNPD24388	[(3Z,5E,8S,9E,11Z,14S,16R,17E,19Z,24R)-14,16-dihydroxy-24-methyl-2-oxo-1-oxacyclotetracosa-3,5,9,11,17,19-hexaen-8-yl] (E,5S)-5-hydroxyhept-3-enoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD25827	N-(3-methylbutyl)tridecanamide		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k

CMNPD25829	(2R)-3-[[(1R,2S,3S,4aS,8aS)-2,3-dihydroxy-5,5,8a-trimethyl-1-[(2E)-3-methylpenta-2,4-dienyl]-3,4,4a,6,7,8-hexahydro-1H-naphthalen-2-yl]methylsulfanyl]-2-acetamidopropanoic acid		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2015;32(2):116-211. doi:10.1039/c4np00144c
CMNPD27172	2-O-(2-methylbutyl) 1-O-propyl benzene-1,2-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2013;30(2):237-323. doi:10.1039/c2np20112g
CMNPD27173	diethyl benzene-1,2-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD27241	4-[[1-[[1-[(1-carboxy-2-hydroxyethyl)amino]-3-hydroxy-1-oxopropan-2-yl]amino]-3-methyl-1-oxobutan-2-yl]amino]-3-[[2-(hexadecanoylamino)-3-hydroxypropanoyl]amino]-4-oxobutanoic acid		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2013;30(2):237-323. doi:10.1039/c2np20112g

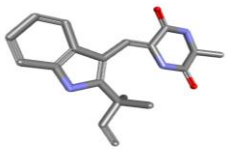
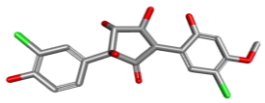
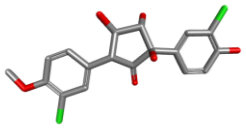
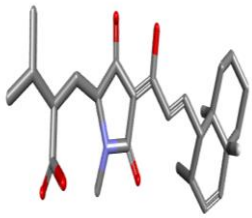
CMNPD28506	5-amino-2-[6-(2-hydroxyethyl)-3-oxononyl]cyclohex-2-en-1-one		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD28507	8-(aminomethyl)-7-hydroxy-1-[1-hydroxy-4-(hydroxymethoxy)-2,3-dimethylbutyl]-2-methyl-2,3,4,4a,4b,5,6,7,8,8a,10,10a-dodecahydro-1H-phenanthren-9-one		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2015;32(2):116-211. doi:10.1039/c4np00144c
CMNPD28508	2-O-[(E)-2-ethylhex-1-enyl] 1-O-[(2E)-2-ethylidenehexyl] cyclohexane-1,2-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2015;32(2):116-211. doi:10.1039/c4np00144c
CMNPD28605	methyl (E)-5-[3-[2-(furan-2-yl)ethyl]-7-hydroxy-4-[(E)-3-methylbut-1-enyl]-3,4,4a,5,6,7,8,8a-octahydro-2H-chromen-6-yl]-4-methylpent-4-enoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2014;31(2):160-258. doi:10.1039/c3np70117d
CMNPD28606	methyl 3-[7-[(E)-1-(furan-2-yl)-3-(hydroxymethyl)-7-methyloct-5-en-4-yl]-3,4,4a,5,6,7,8,8a-octahydronaphthalen-2-yl]propanoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2013;30(2):237-323. doi:10.1039/c2np20112g

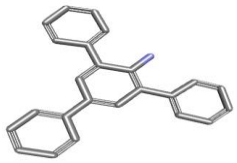
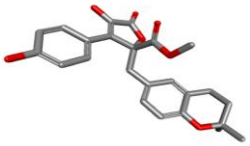
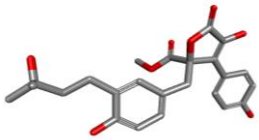
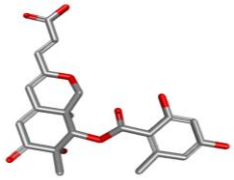
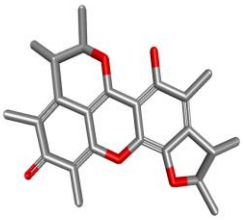
CMNPD28607	methyl 3-[4-[(E)-3-methylpent-1-enyl]-4a,5,6,8,8a,9-hexahydro-4H-furo[3,2-g]isochromen-6-yl]propanoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2012;29(2):144-222. doi:10.1039/c2np00090c
CMNPD28608	8-methoxy-7-(3-methylbutyl)-5a,6,7,8,9,9a-hexahydrobenzo[e][1]benzofuran		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2009;26(2):170-244. doi:10.1039/b805113p
CMNPD28613	[2-methyl-3-(9-propan-2-yl-4a,5,6,8,9,10,10a,10b-octahydro-2H-benzo[h]chromen-4-yl)propyl] benzoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD28614	methyl 8-(2-benzoyloxyethyl)-4-[(E)-pent-2-enyl]-4a,5,6,7,8,8a-hexahydro-2H-chromene-6-carboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD28694	[2-hexadecanoyloxy-3-[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxypropyl] hexadecanoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k

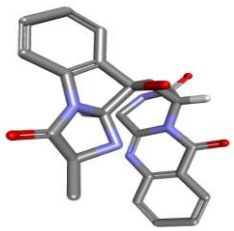
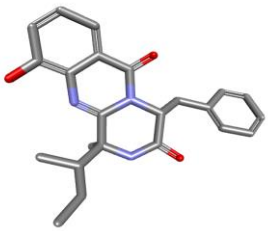
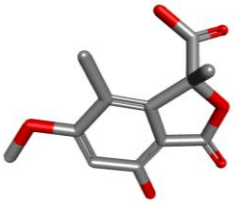
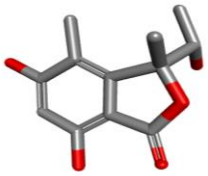
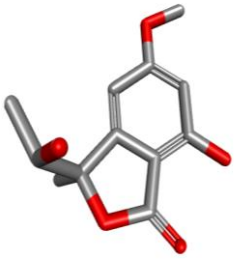
CMNPD29996	[(3Z,5E,9E,11Z,17E,19E)-14,16-dihydroxy-24-methyl-2-oxo-1-oxacyclotetracosa-3,5,9,11,17,19-hexaen-8-yl] 6-(2-acetylphenyl)-5-hydroxyhexanoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD30086	3-[(3R,4S,6S)-4-butyl-6-ethyl-2-oxooxan-3-yl]propyl 2-methylbenzoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD30087	2-[(3R,5S)-2-oxo-5-propan-2-yloxolan-3-yl]ethyl 2-ethoxy-4-hydroxybenzoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD30117	methyl 4,8-dimethylundecanoate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD30237	1-ethenoxy-2-methylbenzene		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156

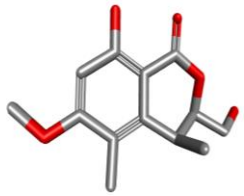
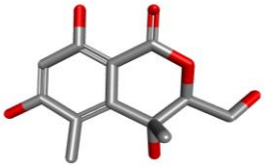
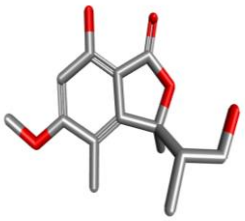
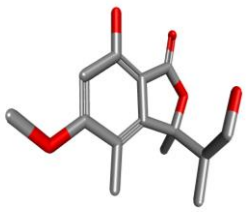
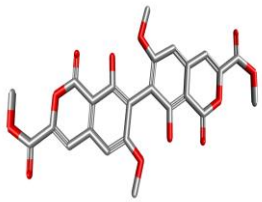
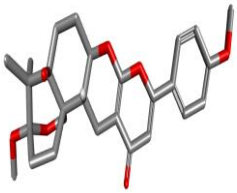
A comprehensive marine natural products database towards facilitating drug discovery from the ocean, Marine organisms are expected to be an important source of inspiration for drug discovery after terrestrial plants and microorganisms. This table contains the bacteria compound name, IUPAC name, structure and reference

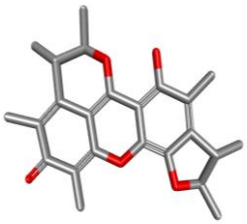
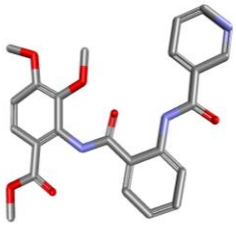
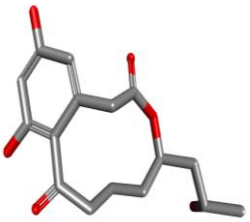
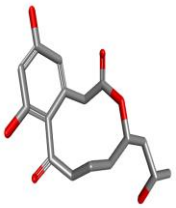
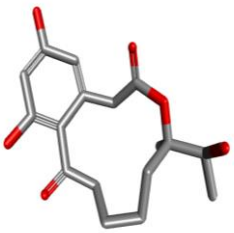
TABLE 5. 2 COMPOUND DETAILS FOR MARINE FUNGI

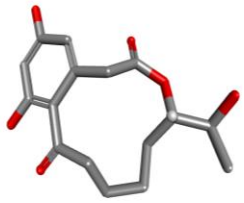
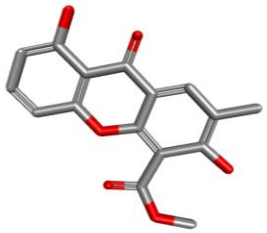
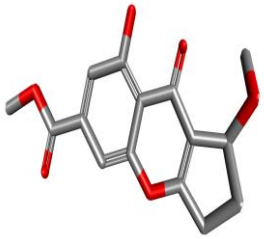
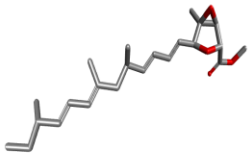
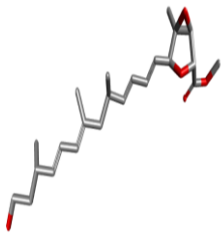
COMPOUND IDENTIFIER	COMPOUND NAME	STRUCTURE	REFERENCE
CMNPD22236	(6Z)-3-methyl-6-[[2-(2-methylbut-3-en-2-yl)-1H-indol-3-yl]methylidene]piperazine-2,5-dione		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2014 Jan 17;31(2):160-258. doi: 10.1039/24389707 24389707.
CMNPD15724	5-(5-chloro-2-hydroxy-4-methoxyphenyl)-2-(3-chloro-4-hydroxyphenyl)-2,3,4-trihydroxycyclopentan-1-one		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2008 Feb;25(1):35-94. doi: 10.1039/b701534h. Epub 2008 Jan 3. PMID: 18250897.
CMNPD15725	2-(3-chloro-4-hydroxyphenyl)-5-(3-chloro-4-methoxyphenyl)-2,3,4-trihydroxycyclopentan-1-one		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2008 Feb;25(1):35-94. doi: 10.1039/b701534h. Epub 2008 Jan 3. PMID: 18250897.
CMNPD12450	2-[[4-[(E)-3-[(1S,2S,4aR,8aS)-2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]-1-hydroxyprop-2-enylidene]-1-methyl-3,5-dioxopyrrolidin-2-yl]methyl]-2-hydroxy-3-methylbutanoic acid		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD12451	2-[[4-[(E)-3-[(1S,2S,4aR,8aS)-2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]-1-hydroxyprop-2-enylidene]-1-methyl-3,5-dioxopyrrolidin-2-yl]methyl]-2-hydroxy-3-methylpentanoic acid		Blunt JW, Copp BR, Keyzers RA, Munro MHG, Prinsep MR. Marine natural products. Nat Prod Rep. 2017 Mar 17;34(3):235-294. doi: 10.1039/c6np00124f. PMID: 28290569.

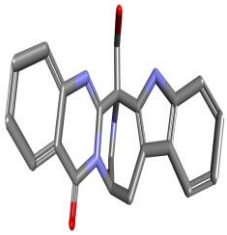
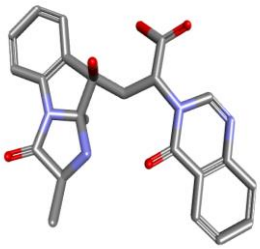
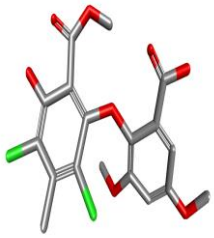
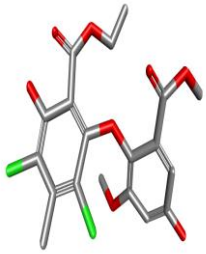
CMNPD30821	2,4,6-triphenylaniline		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD18724	methyl (2R)-2-[(2,2-dimethyl-3,4-dihydrochromen-6-yl)methyl]-4-hydroxy-3-(4-hydroxyphenyl)-5-oxofuran-2-carboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MHG, Prinsep MR. Marine natural products. Nat Prod Rep. 2017 Mar 17;34(3):235-294. doi: 10.1039/c6np00124f. PMID: 28290569.
CMNPD18725	methyl (2R)-4-hydroxy-2-[[4-hydroxy-3-(3-hydroxy-3-methylbutyl)phenyl]methyl]-3-(4-hydroxyphenyl)-5-oxofuran-2-carboxylate		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2011 Feb;28(2):196-268. doi: 10.1039/c005001f. Epub 2010 Dec 13. PMID: 21152619.
CMNPD28911	(E)-3-[(7S,8S,8aS)-8-(2,4-dihydroxy-6-methylbenzoyl)oxy-7-hydroxy-7-methyl-6-oxo-8,8a-dihydro-1H-isochromen-3-yl]prop-2-enoic acid		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD25904	methyl (2R)-7-hydroxy-8-methoxy-2-methyl-4-oxo-3,5-dihydro-2H-pyrano[3,2-c]chromene-10-carboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MHG, Prinsep MR. Marine natural products. Nat Prod Rep. 2017 Mar 17;34(3):235-294. doi: 10.1039/c6np00124f. PMID: 28290569.

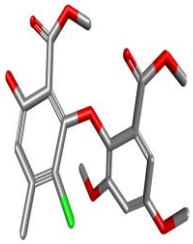
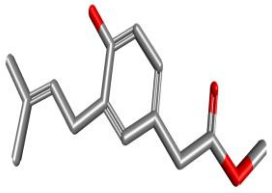
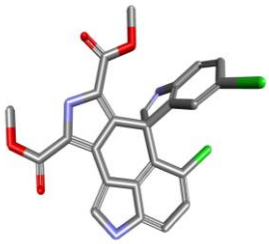
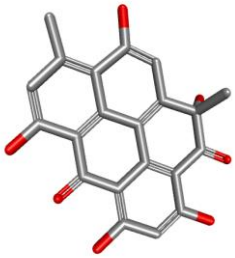
CMNPD26113	(4R)-4-[[(2S,3aS,4R)-4-hydroxy-2-methyl-1-oxo-3,3a-dihydro-2H-imidazo[1,2-a]indol-4-yl]methyl]-2,4-dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-dione		Blunt JW, Copp BR, Keyzers RA, Munro MHG, Prinsep MR. Marine natural products. Nat Prod Rep. 2017 Mar 17;34(3):235-294. doi: 10.1039/c6np00124f. PMID: 28290569.
CMNPD26114	(1S,4R)-4-benzyl-1-butan-2-yl-10-hydroxy-2,4-dihydro-1H-pyrazino[2,1-b]quinazoline-3,6-dione		Blunt JW, Copp BR, Keyzers RA, Munro MHG, Prinsep MR. Marine natural products. Nat Prod Rep. 2017 Mar 17;34(3):235-294. doi: 10.1039/c6np00124f. PMID: 28290569.
CMNPD28880	(1R)-4-hydroxy-6-methoxy-1,7-dimethyl-3-oxo-2-benzofuran-1-carboxylic acid		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28881	(3R)-5,7-dihydroxy-3-[(1S)-1-hydroxyethyl]-3,4-dimethyl-2-benzofuran-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28882	(3R)-7-hydroxy-3-[(1S)-1-hydroxyethyl]-5-methoxy-3-methyl-2-benzofuran-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.

CMNPD28883	(3R,4S)-8-hydroxy-3-(hydroxymethyl)-6-methoxy-4,5-dimethyl-3,4-dihydroisochromen-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28884	(3S,4R)-4,6,8-trihydroxy-3-(hydroxymethyl)-4,5-dimethyl-3H-isochromen-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28885	(3S)-7-hydroxy-3-[(2S)-1-hydroxypropan-2-yl]-5-methoxy-3,4-dimethyl-2-benzofuran-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28886	(3S)-7-hydroxy-3-[(2R)-1-hydroxypropan-2-yl]-5-methoxy-3,4-dimethyl-2-benzofuran-1-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28902	methyl 8-hydroxy-7-(8-hydroxy-6-methoxy-3-methoxycarbonyl-1-oxoisochromen-7-yl)-6-methoxy-1-oxoisochromene-3-carboxylate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28903	(1R,2R,11R,14S,16S)-14-hydroxy-16-methoxy-7-(4-methoxyphenyl)-11,15,15-trimethyl-8,10,17-trioxapentacyclo[14.2.2.01,14.02,11.04,9]icosa-4(9),6-dien-5-		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub

	one		2019 Jan 21. PMID: 30663727.
CMNPD28904	(6S,7R,17S,18R)-3-hydroxy-4,6,7,13,15,17,18-heptamethyl-8,11,19-trioxapentacyclo[10.7.1.02,10.05,9.016,20]icosa-1(20),2,4,9,12,15-hexaen-14-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28906	4-[(E)-prop-1-enyl]-2,3-dihydropyran-6-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28931	(4R)-9,11-dihydroxy-4-[(2S)-2-hydroxypropyl]-4,5,6,7-tetrahydro-1H-3-benzoxecine-2,8-dione		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28932	(4S)-9,11-dihydroxy-4-[(2S)-2-hydroxypropyl]-4,5,6,7-tetrahydro-1H-3-benzoxecine-2,8-dione		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28933	(5R)-12,14-dihydroxy-5-[(1S)-1-hydroxyethyl]-4-oxabicyclo[9.4.0]pentadeca-1(15),11,13-triene-3,10-dione		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.

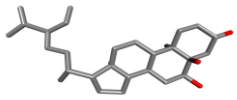
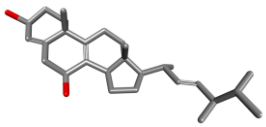
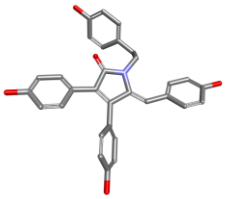
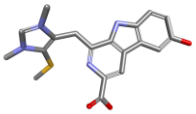
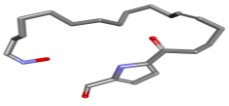
CMNPD28934	(5S)-12,14-dihydroxy-5-[(1S)-1-hydroxyethyl]-4-oxabicyclo[9.4.0]pentadeca-1(15),11,13-triene-3,10-dione		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28965	methyl 3,8-dihydroxy-2-methyl-9-oxoxanthene-4-carboxylate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD28966	methyl 8-hydroxy-1-methoxy-9-oxo-2,3-dihydro-1H-cyclopenta[b]chromene-6-carboxylate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD29067	methyl (1S,2R,4S,5R)-5-methyl-4-[(1E,3E,5R,7E,9E,11S)-5,7,11-trimethyltrideca-1,3,7,9-tetraenyl]-3,6-dioxabicyclo[3.1.0]hexane-2-carboxylate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD29068	methyl (1S,2R,4S,5R)-4-[(1E,3E,5R,7E,9E,11S)-13-hydroxy-5,7,11-trimethyltrideca-1,3,7,9-tetraenyl]-5-methyl-3,6-dioxabicyclo[3.1.0]hexane-2-carboxylate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.

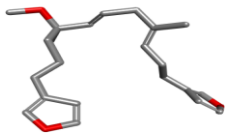
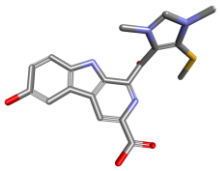
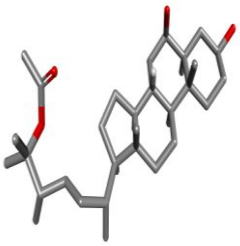
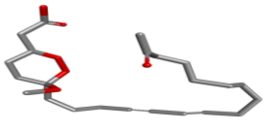
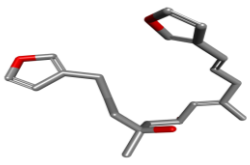
CMNPD29070	(2R,3S)-3-hydroxy-3-methyl-2-[(1E,3E,5R,7E,9E,11S)-5,7,11-trimethyltrideca-1,3,7,9-tetraenyl]-2H-pyran-6-one		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2019 Jan 1;36(1):122-173. doi: 10.1039/c8np00092a. Epub 2019 Jan 21. PMID: 30663727.
CMNPD30304	(1R,12S)-1-(hydroxymethyl)-3,13,21,23-tetrazahexacyclo[10.10.2.02,10.04,9.013,22.015,20]tetracosa-2(10),4(9),5,7,15,17,19,21-octaene-14,24-dione		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD30305	(2R)-3-[(2S,3aS,4S)-4-hydroxy-2-methyl-1-oxo-3,3a-dihydro-2H-imidazo[1,2-a]indol-4-yl]-2-(4-oxoquinazolin-3-yl)propanoic acid		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD30637	2-(2,4-dichloro-5-hydroxy-6-methoxycarbonyl-3-methylphenoxy)-3,5-dimethoxybenzoic acid		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD30638	ethyl 3,5-dichloro-2-hydroxy-6-(4-hydroxy-2-methoxy-6-methoxycarbonylphenoxy)-4-methylbenzoate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.

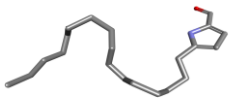
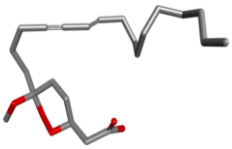
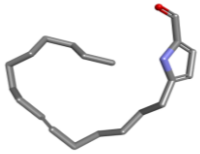
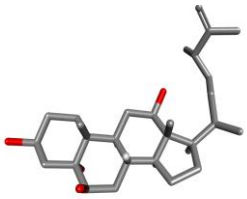
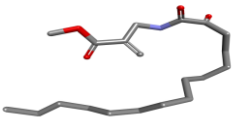
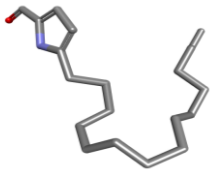
CMNPD30639	methyl 3-chloro-2-(2,4-dimethoxy-6-methoxycarbonylphenoxy)-6-hydroxy-4-methylbenzoate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD30643	methyl 2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]acetate		Carroll AR, Copp BR, Davis RA, Keyzers RA, Prinsep MR. Marine natural products. Nat Prod Rep. 2020 Feb 26;37(2):175-223. doi: 10.1039/c9np00069k. PMID: 32025684.
CMNPD21959	dimethyl (7S)-5',9-dichlorospiro[4,13-diazatetracyclo[6.6.1.02,6.012,15]pentadeca-1(14),2,5,8(15),9,11-hexaene-7,3'-indole]-3,5-dicarboxylate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2014 Jan 17;31(2):160-258. doi: 10.1039/c3np70117d. PMID: 24389707.
CMNPD14698	2,4,7,10,14-pentahydroxy-7,12-dimethylpentacyclo[13.3.1.05,18.08,17.011,16]nonadeca-1,3,5(18),8(17),9,11,13,15-octaene-6,19-dione		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2007 Feb;24(1):31-86. doi: 10.1039/b603047p. Epub 2007 Jan 11. PMID: 17268607.

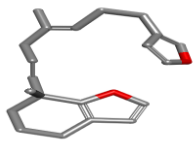
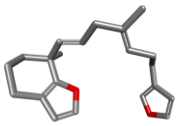
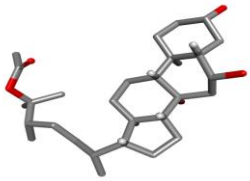
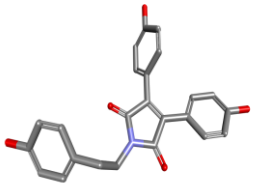
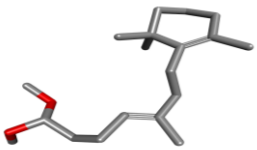
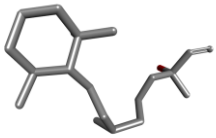
A comprehensive marine natural products database towards facilitating drug discovery from the ocean, Marine organisms are expected to be an important source of inspiration for drug discovery after terrestrial plants and microorganisms. This table contains the fungi compound name, IUPAC name, structure and reference

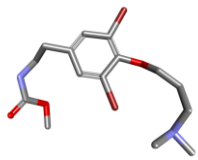
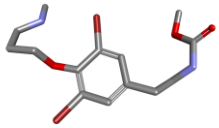
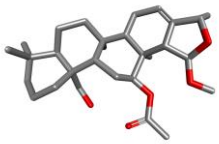
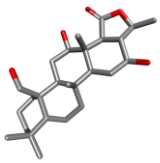
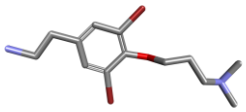
TABLE 5.3 COMPOUND DETAILS FOR MARINE SPONGES

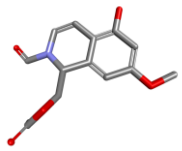
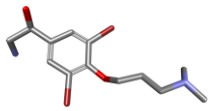
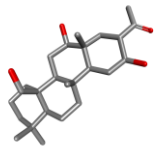
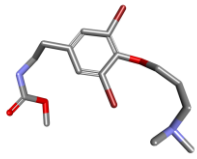
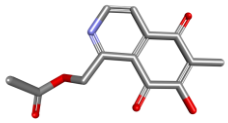
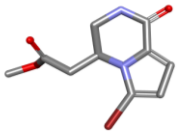
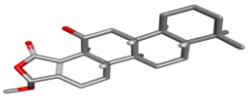
COMPOUND IDENTIFIER	COMPOUND NAME	STRUCTURE	REFERENCE
CMNPD6261	(3S,5R,6S,10R,13R,17R)-17-[(2R,5S)-5-ethyl-6-methylheptan-2-yl]-10,13-dimethyl-1,2,3,4,6,7,8,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthrene-3,5,6-triol		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2006 Feb;23(1):26-78. doi: 10.1039/b502792f. Epub 2006 Jan 9. PMID: 16453031.
CMNPD8365	(7-hydroxy-6-methyl-5,8-dioxoisoquinolin-1-yl)methyl (Z)-2-methylbut-2-enoate		Faulkner DJ. Marine natural products. Nat Prod Rep. 1998 Apr;15(2):113-58. doi: 10.1039/a815113y. PMID: 9586223.
CMNPD25206	(5Z)-3,4-bis(4-hydroxyphenyl)-1-[2-(4-hydroxyphenyl)ethyl]-5-[(4-hydroxyphenyl)methylidene]pyrrol-2-one		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2016 Mar;33(3):382-431. doi: 10.1039/c5np00156k. Epub 2016 Feb 3. PMID: 26837534.
CMNPD14213	dragmacidonamine B		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2006 Feb;23(1):26-78. doi: 10.1039/b502792f. Epub 2006 Jan 9. PMID: 16453031.
CMNPD11118	Mycaleoxime		Faulkner DJ. Marine natural products. Nat Prod Rep. 1998 Apr;15(2):113-58. doi: 10.1039/a815113y. PMID: 9586223.

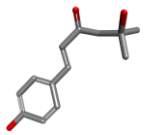
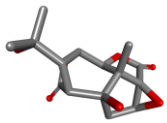
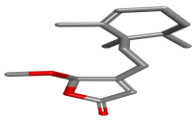
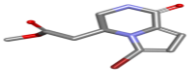
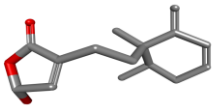
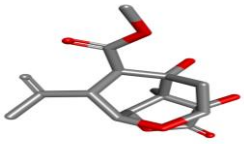
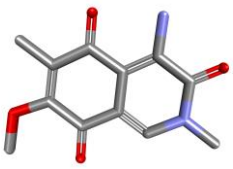
CMNPD5569	3-[(3E,7E)-11-(furan-3-yl)-6-methoxy-4,8-dimethylundeca-3,7-dienyl]furan		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019.
CMNPD5568	3-[(3E,6E)-11-(furan-3-yl)-8-methoxy-4,8-dimethylundeca-3,6-dienyl]furan		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019.
CMNPD14212	dragmacidonamine A		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2006 Feb;23(1):26-78. doi: 10.1039/b502792f. Epub 2006 Jan 9. PMID: 16453031.
CMNPD20295	[(3S,6R)-6-[(3S,5S,6R,8S,9S,10R,13R,14S,17R)-3,6-dihydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]-2,3-dimethylheptan-2-yl] acetate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2012 Feb;29(2):144-222. doi: 10.1039/c2np00090c. Epub 2011 Dec 22. PMID: 22193773.
CMNPD11843	peroxyacarnoic acid C		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019
CMNPD11249	untenospongin A		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019

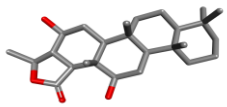
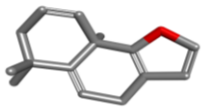
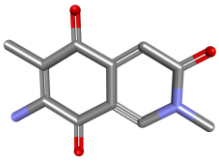
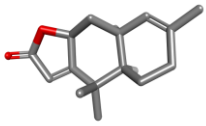
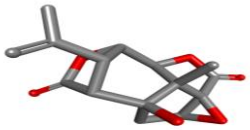
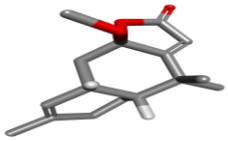
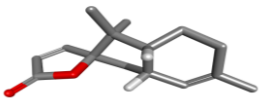
CMNPD967	2-formyl-5-hexadecylpyrrol		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2012 Feb;29(2):144-222. doi: 10.1039/c2np00090c. Epub 2011 Dec 22.
CMNPD11844	peroxyacarnoic acid D		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431.
CMNPD11119	(6′E)-5-(pentadec-6′-enyl)pyrrole-2-carbaldehyde		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431.
CMNPD20297	(3S,5R,6R,8S,9S,10R,12R,13R,14S,17R)-17-[(2R,5S)-5,6-dimethylhept-6-en-2-yl]-10,13-dimethyl-1,2,3,4,6,7,8,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthrene-3,5,6,12-tetrol		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2012 Feb;29(2):144-222. doi: 10.1039/c2np00090c. Epub 2011 Dec 22. PMID: 22193773.
CMNPD878	methyl 2-[(2-oxopentadecanoylamino)methyl]prop-2-enoate		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019.
CMNPD966	5-pentadecyl-1H-pyrrole-2-carbaldehyde		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2012 Feb;29(2):144-222. doi: 10.1039/c2np00090c. Epub 2011 Dec 22. PMID:

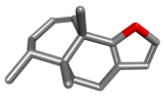
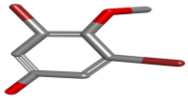
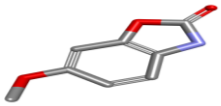
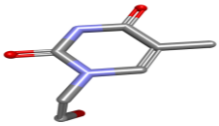
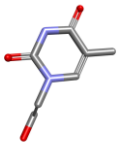
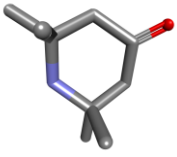
			22193773.
CMNPD5567	7-[(1E,4E)-7-(furan-3-yl)-4-methylhepta-1,4-dienyl]-7-methyl-5,6-dihydro-4H-1-benzofuran		Faulkner DJ. Marine natural products. Nat Prod Rep. 1994 Aug;11(4):355-94. doi: 10.1039/np9941100355. PMID: 15200019.
CMNPD8324	(7S)-7-[(1E,4E)-7-(furan-3-yl)-4-methylhepta-1,4-dienyl]-7-methyl-5,6-dihydro-4H-1-benzofuran		Faulkner DJ. Marine natural products. Nat Prod Rep. 1998 Apr;15(2):113-58. doi: 10.1039/a815113y. PMID: 9586223.
CMNPD20296	[(3S,6R)-2,3-dimethyl-6-[(3S,5S,6R,8R,9R,10S,13R,14R,17R)-3,6,8-trihydroxy-10,13-dimethyl-1,2,3,4,5,6,7,9,11,12,14,15,16,17-tetradecahydrocyclopenta[a]phenanthren-17-yl]heptan-2-yl] acetate		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2012 Feb;29(2):144-222. doi: 10.1039/c2np00090c. Epub 2011 Dec 22. PMID: 22193773.
CMNPD25205	denigrin A		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. Nat Prod Rep. 2016 Mar;33(3):382-431. doi: 10.1039/c5np00156k. Epub 2016 Feb 3. PMID: 26837534.
CMNPD6896	trisnorditerpene		Faulkner DJ. Marine natural products. Nat Prod Rep. 1996 Apr;13(2):75-125. doi: 10.1039/np9961300075. PMID: 8622813.
CMNPD7692	25-dehydroxy-12-epi-deacetylscalarin		Faulkner DJ. Marine natural products. Nat Prod Rep. 1996 Apr;13(2):75-125. doi: 10.1039/np9961300075. PMID: 8622813.

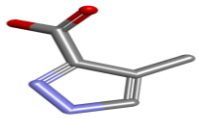
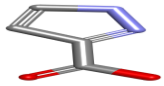
CMNPD10435	methyl N-[2-[3,5-dibromo-4-[3-(dimethylamino)propoxy]phenyl]ethyl]carbamate		Faulkner DJ. Marine natural products. Nat Prod Rep. 1998 Apr;15(2):113-58. doi: 10.1039/a815113y. PMID: 9586223.
CMNPD15143	methyl N-[2-[3,5-dibromo-4-[3-(methylamino)propoxy]phenyl]ethyl]carbamate		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2007 Feb;24(1):31-86. doi: 10.1039/b603047p. Epub 2007 Jan 11. PMID: 17268607.
CMNPD6245	22-hydroxy-25-methoxy-24-methyldeoxoscalarin		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2007 Feb;24(1):
CMNPD11117	(6′Z)-5-(23′-cyanotricos-6′-enyl)pyrrole-2-carbaldehyde		Kiran GS, Yang YH, Selvin J. Marine sponge-associated bacteria as a potential source for polyhydroxyalkanoates. Crit Rev Microbiol. 2017 May;43(3):294-312. doi: 10.1080/1040841X.2016.1206060. Epub 2016 Nov 8. PMID: 27824282
CMNPD5010	12β,16β,22-trihydroxy-24-methylscalaran-25,24-olide		Faulkner DJ. Marine natural products. Nat Prod Rep. 1993 Oct;10(5):497-539. doi: 10.1039/np9931000497. PMID: 8295744.
CMNPD9619	purpurealidin E		Faulkner DJ. Marine natural products. Nat Prod Rep. 2000 Feb;17(1):7-55. doi: 10.1039/a809395d. PMID: 10714898.

CMNPD10387	1,2-dihydroisoquinoline		Blunt JW, Copp BR, Hu WP, Munro MH, Northcote PT, Prinsep MR. Marine natural products. Nat Prod Rep. 2007 Feb;24(1):
CMNPD14268	(2R,5S,7S,9R,15R,16S)-15-[(1S)-1-[(2R)-5-hydroxy-4-(2-hydroxypropan-2-yl)oxolan-2-yl]ethyl]-2,16-dimethyl-8-oxapentacyclo[9.7.0.02,7.07,9.012,16]octadecan-5-ol		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD5012	12β,16β,22-trihydroxy-24-methyl-24-oxo-25-norscalarae		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497
CMNPD6716	3α-methylaraguspongine C		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD6139	isoquinolinequinone		Kiran GS, Yang YH, Selvin J. Marine sponge-associated bacteria as a potential source for polyhydroxyalkanoates. Crit Rev Microbiol. 2017 May;43(3):294-312. doi:.
CMNPD11153	ambliol B †		Faulkner DJ. Marine natural products. Nat Prod Rep. 1993 Oct;10(5):497-539. doi: 10.1039/np9931000497. PMID: 8295744
CMNPD18101	24β-methoxyscalarolide		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2010;27(2):165-237. doi:10.1039/b906091j

CMNPD7623	phycopsisenone		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD2772	picrotin		Blunt JW, Copp BR, Munro MH, Northcote PT, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2010;27(2):165-237. doi:10.1039/b906091j
CMNPD9738	furanosesquiterpene		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 2000;17(1):7-55. doi:10.1039/a809395d
CMNPD11153	(S)-(+)-hanashin methyl ester		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497
CMNPD6877	4-[2-[(1R,6R)-1,6-dimethyl-2-methylidenecyclohex-3-en-1-yl]ethyl]-2-hydroxy-2H-furan-5-one		Faulkner DJ. Marine natural products. Nat Prod Rep. 1996 Apr;13(2):75-125. doi: 10.1039/np9961300075. PMID: 8622813.
CMNPD2773	methyl (1S,2S,6R,7R,9S,10S,11R)-1,6-dihydroxy-2-methyl-5-oxo-10-prop-1-en-2-yl-4,8-dioxatetracyclo[5.4.1.02,6.03,9]dodecane-11-carboxylate		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD6756	4-aminomimosamysin		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075

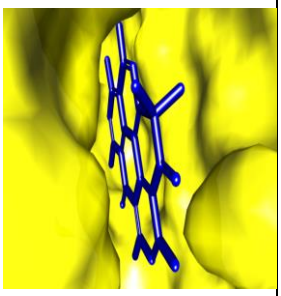
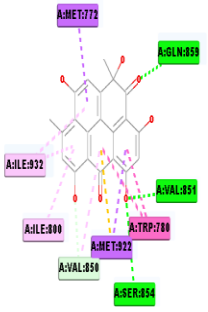
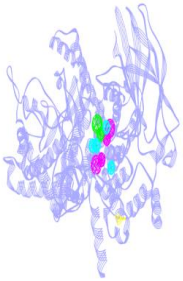
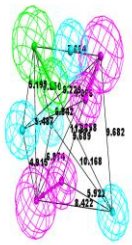
CMNPD5011	12β,16β-dihydroxy-24-methylscalaran-25,24-olide		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497
CMNPD6875	axinellin-B		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD6757	7-amino-7-demethoxymimosamycin		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD1065	furodysinin lactone		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD2771	picrotoxinin		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD3038	O-methylfurodysinin lactone		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD11223	spirofragilide		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075

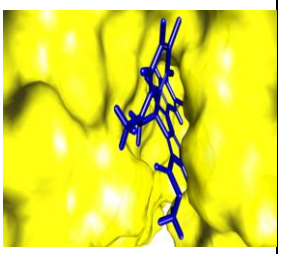
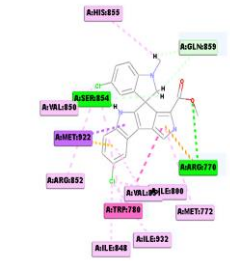
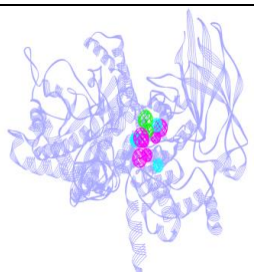
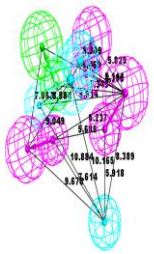
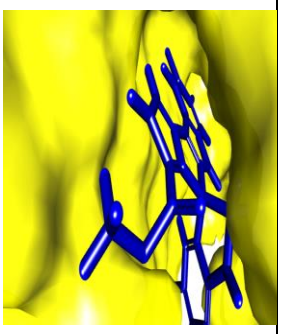
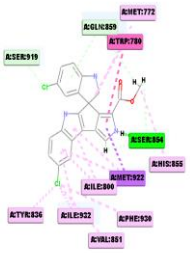
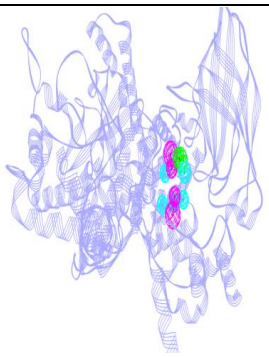
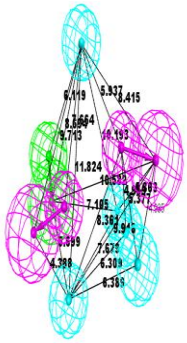
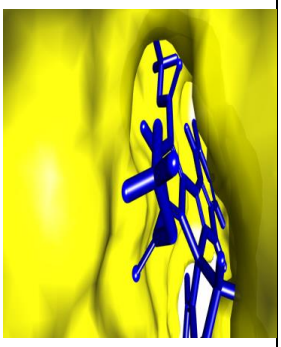
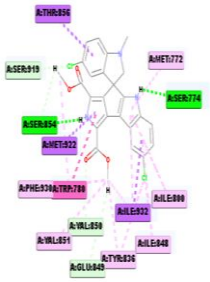
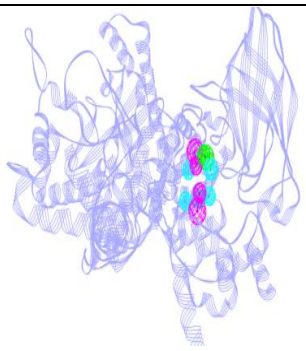
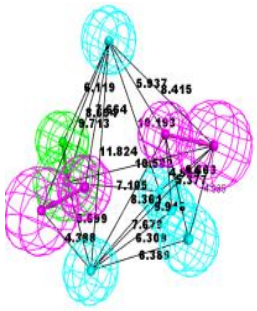
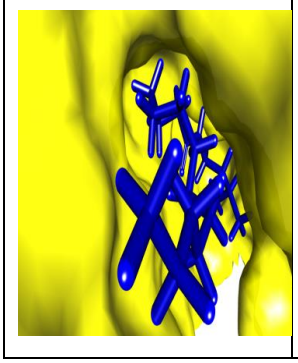
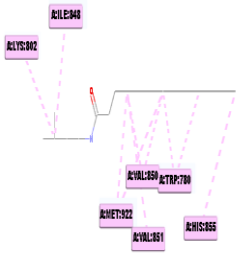
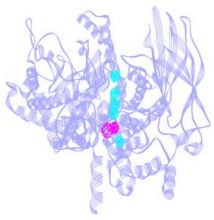
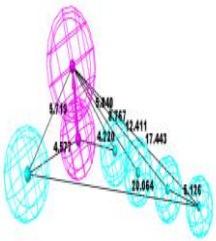
CMNPD2769	herbacin		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431.
CMNPD6876	3,5-dibromo-4-methoxyphenol		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD10459	coixol		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497
CMNPD25208	cis-thyminenol		Blunt JW, Copp BR, Keyzers RA, Munro MH, Prinsep MR. Marine natural products. *Nat Prod Rep*. 2016;33(3):382-431. doi:10.1039/c5np00156k
CMNPD6874	axinellin-A		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD25209	trans-thyminenol		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075
CMNPD5149	acetone (+ammonia) trimer		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497

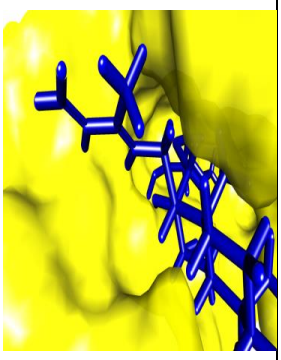
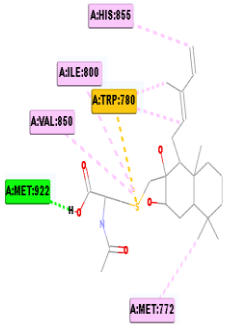
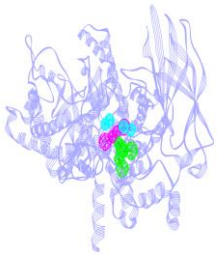
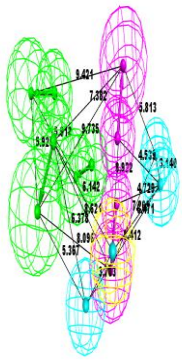
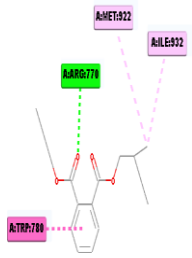
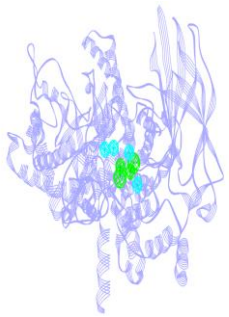
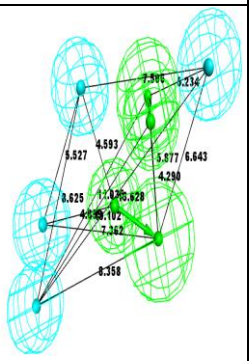
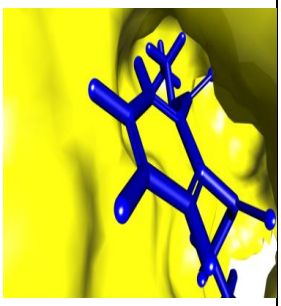
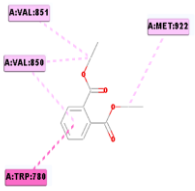
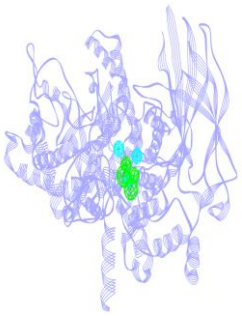
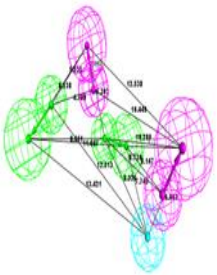
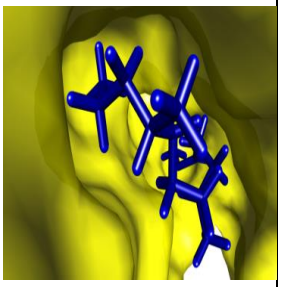
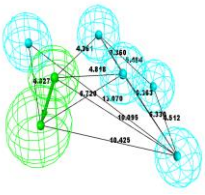
CMNPD8982	4-methylpyrazole-3(5)-carboxylic acid		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1993;10(5):497-539. doi:10.1039/np9931000497
CMNPD8981	pyrazole-3(5)-carboxylic acid		Faulkner DJ. Marine natural products. *Nat Prod Rep*. 1996;13(2):75-125. doi:10.1039/np9961300075

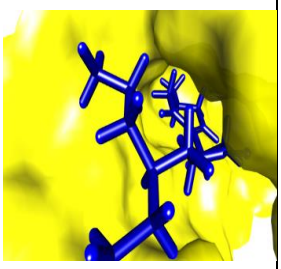
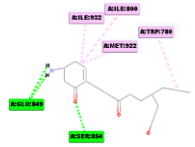
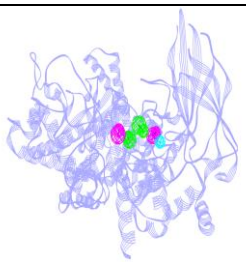
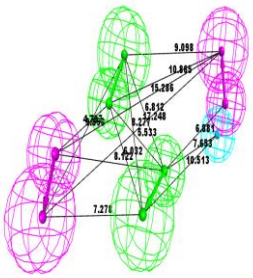
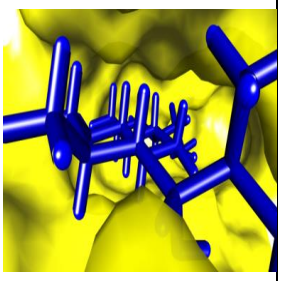
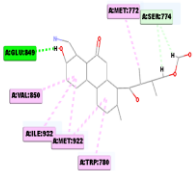
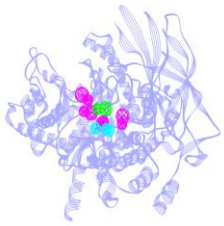
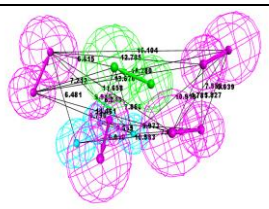
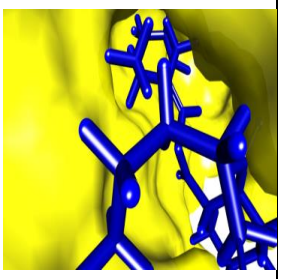
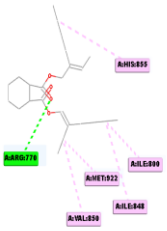
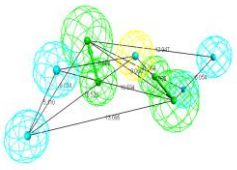
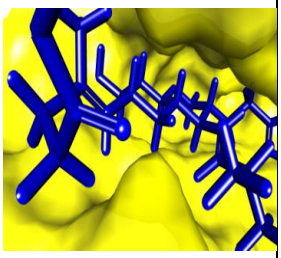
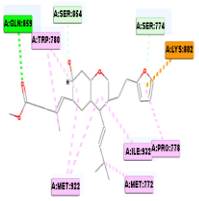
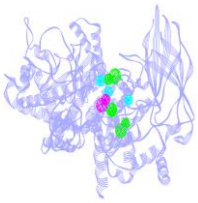
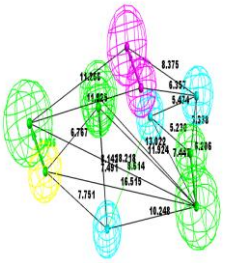
A comprehensive marine natural products database towards facilitating drug discovery from the ocean, Marine organisms are expected to be an important source of inspiration for drug discovery after terrestrial plants and microorganisms. This table contains the sponges compound name, IUPAC name, structure and reference.

TABLE 5.4 2D ,3D STRUCTURE , PHARMACOPHORE AND GEOMETRY FOR MARINE BACTERIA

SURFACE NAME	2D STRUCTURE	PHARMACOPHORE STRUCTURE	GEOMETRY
CMNPD14698 			

CMNPD21959 			
CMNPD21961 			
CMNPD21962 			
CMNPD25827 			

CMNPD25829 			
CMNPD27172 			
CMNPD27173 			
CMNPD27241 			

CMNPD28506 			
CMNPD28507 			
CMNPD28508 			
CMNPD28605 			

This table contains surface name, 2d structure, pharmacophore, geometry distance and structure (ligand interaction) Molecular docking of ligand and target. This figure indicates 3D and 2D interaction between target proteins a Triparanol interaction with 11βHSD.The pharmacophore features colors coded as cyan hydrophobic (HY), orange ring aromatic (RA) green hydrogen bond acceptor (HBA).

TABLE 5.5 2D ,3D STRUCTURE , PHARMACOPHORE AND GEOMETRY FOR MARINE FUNGI

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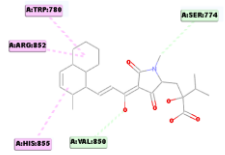
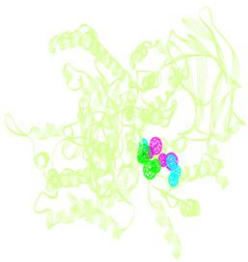
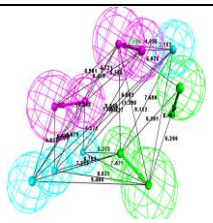
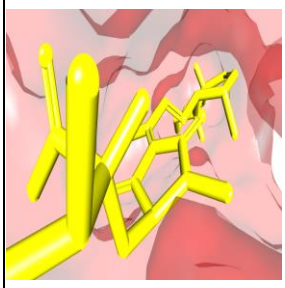
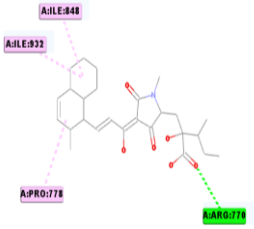
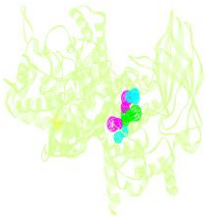
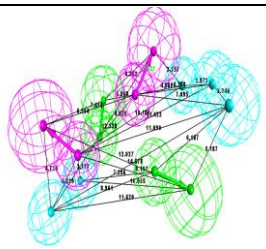
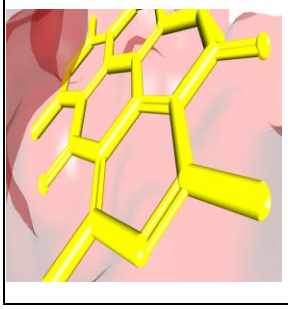
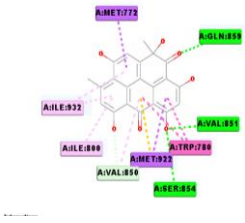
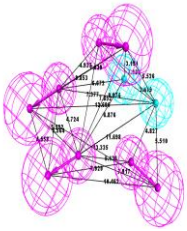
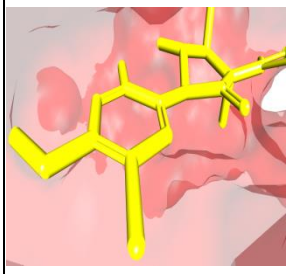
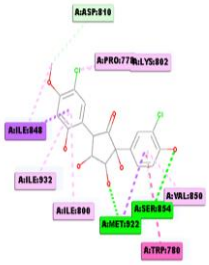
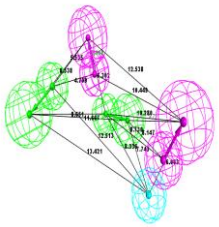
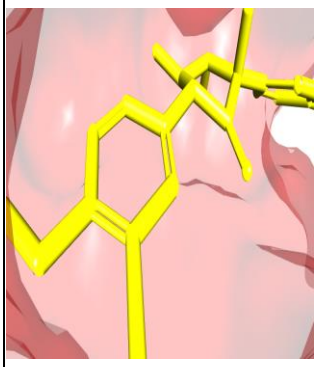
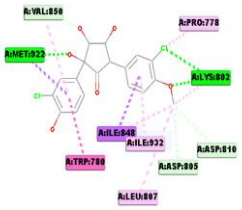
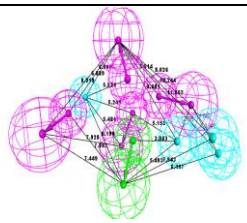
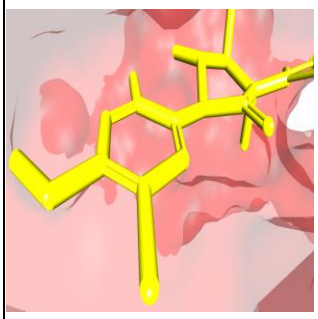
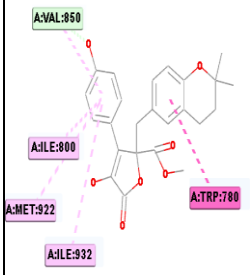
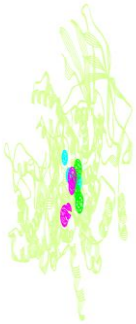
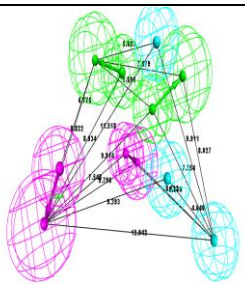
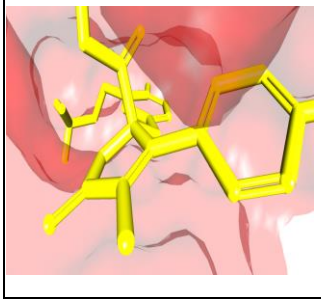
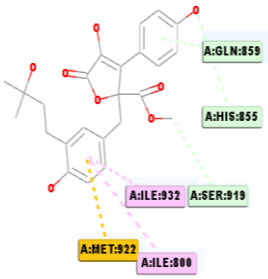
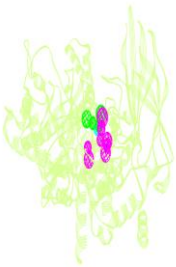
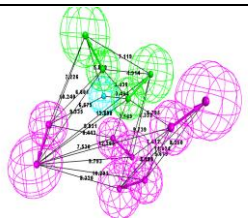
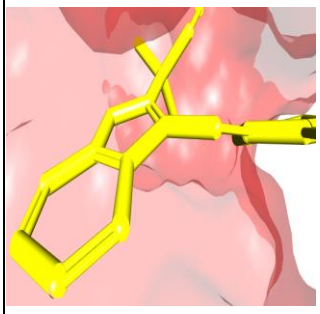
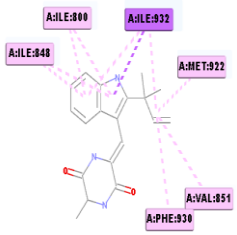
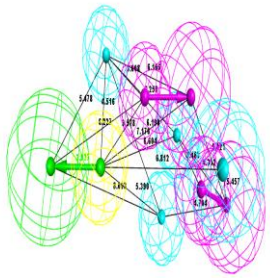
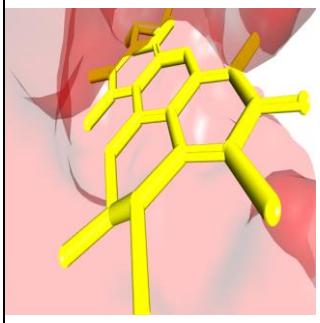
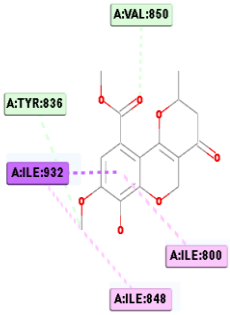
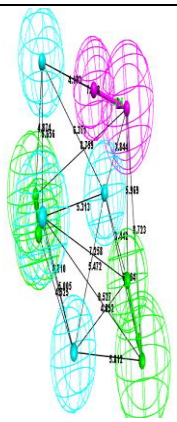
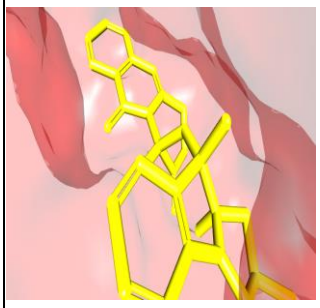
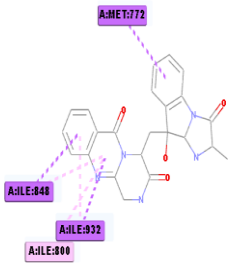
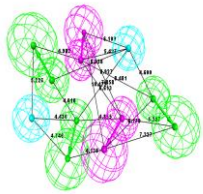
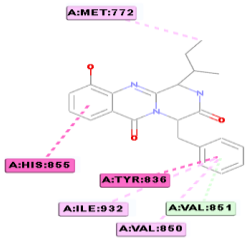
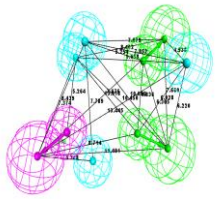
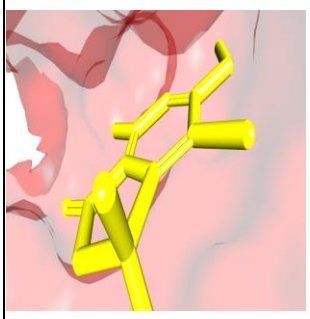
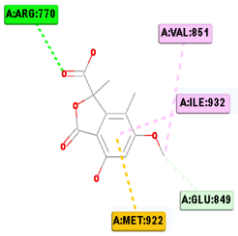
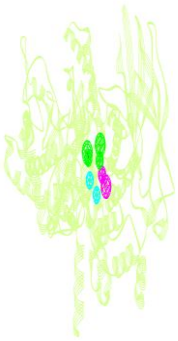
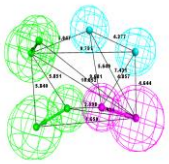
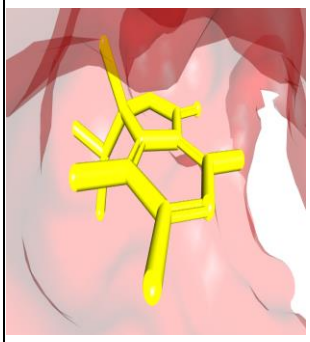
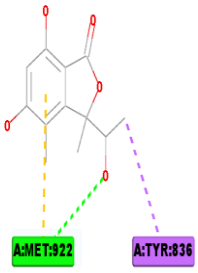
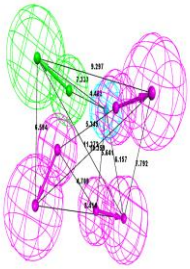
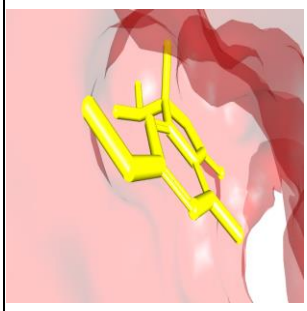
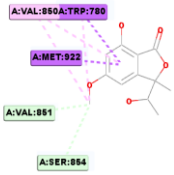
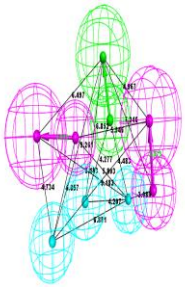
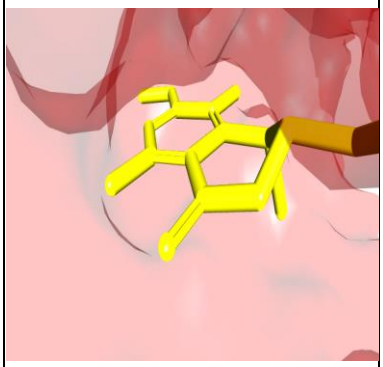
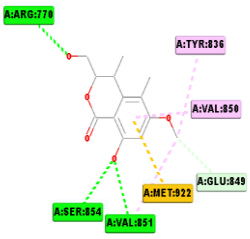
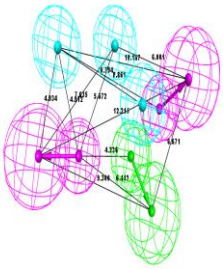
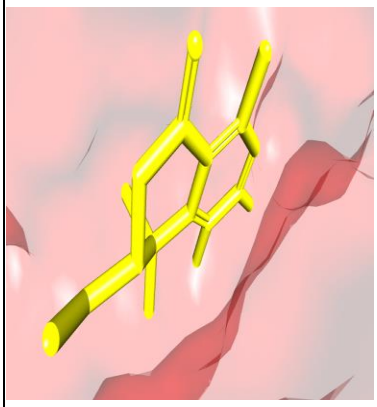
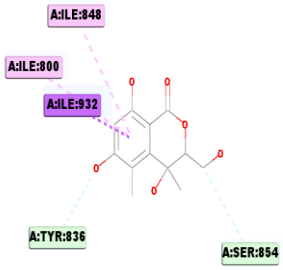
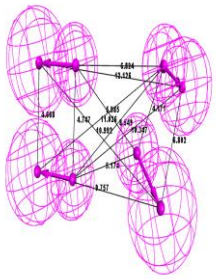
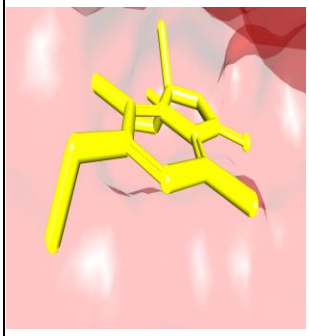
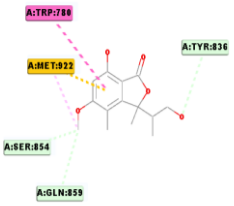
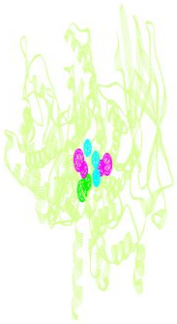
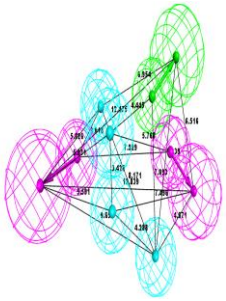
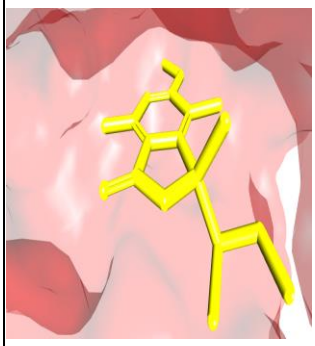
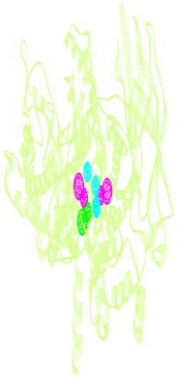
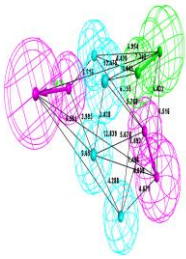
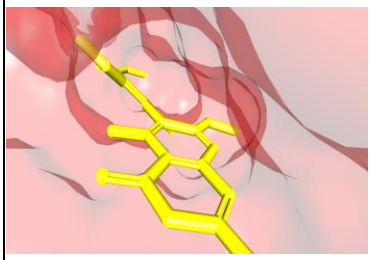
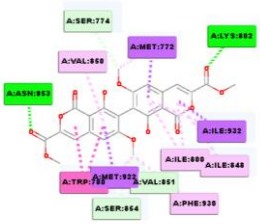
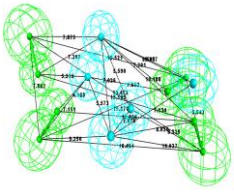
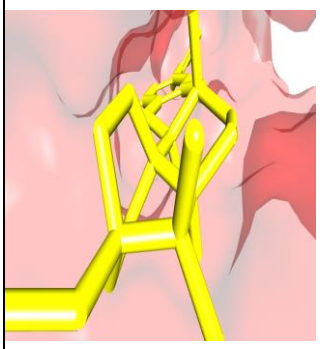
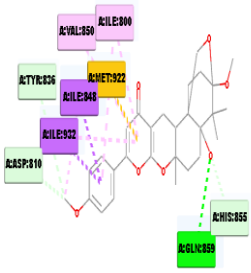
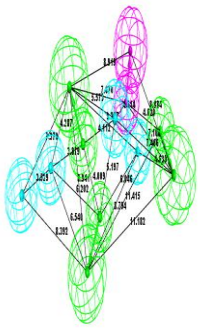
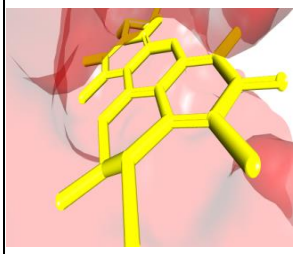
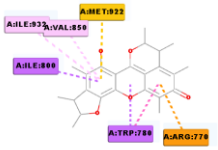
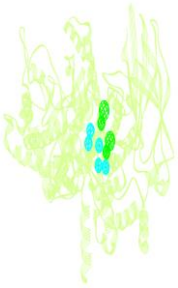
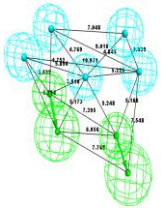
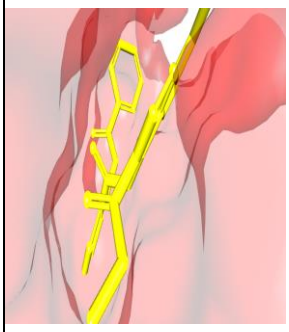
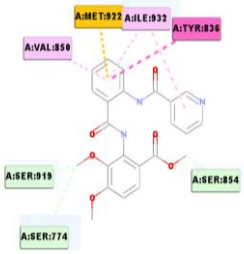
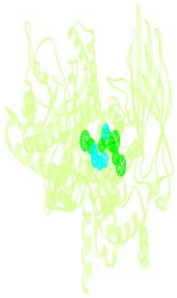
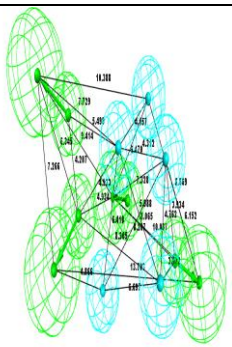
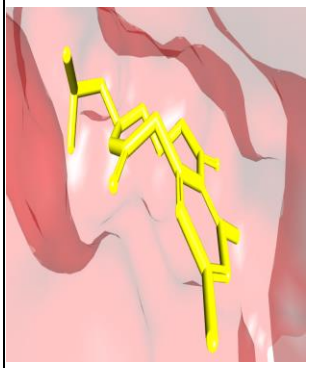
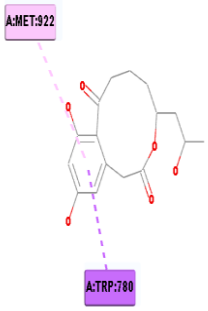
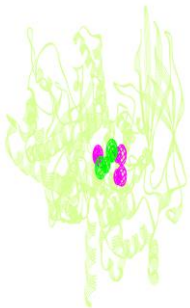
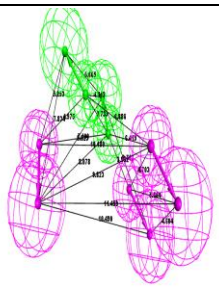
CMNPD12450 			
CMNPD12451 			
CMNPD14698 			

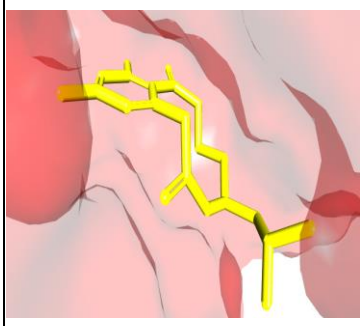
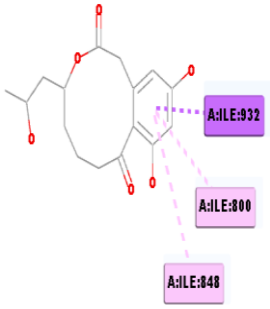
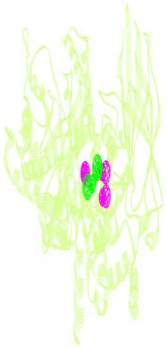
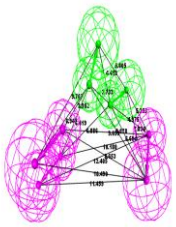
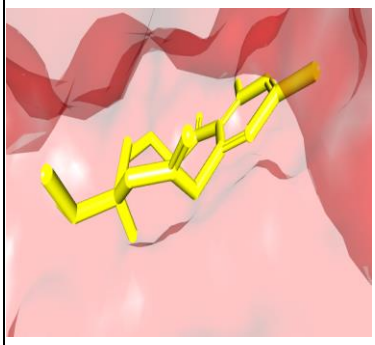
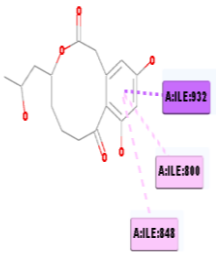
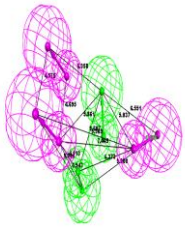
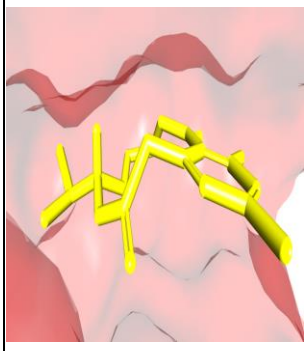
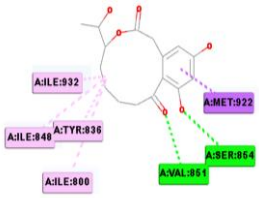
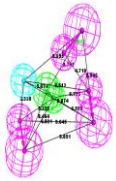
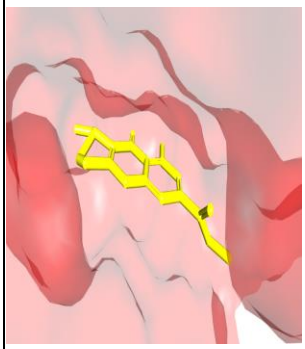
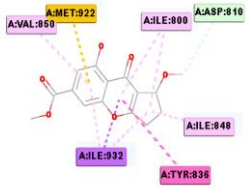
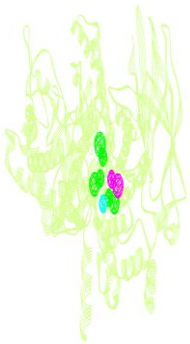
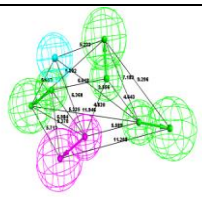
CMNPD15724 			
CMNPD15725 			
CMNPD18724 			
CMNPD18725 			

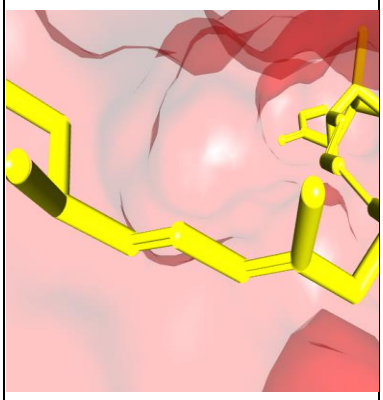
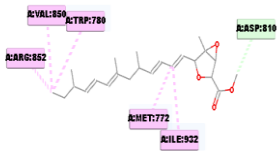
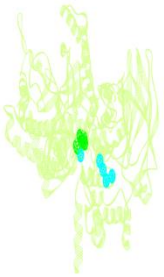
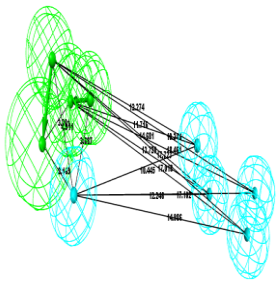
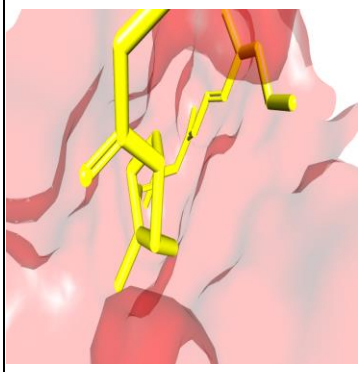
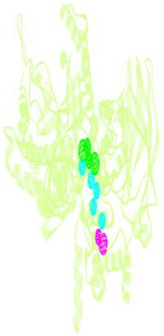
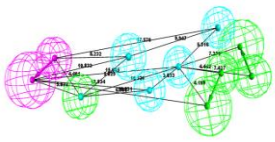
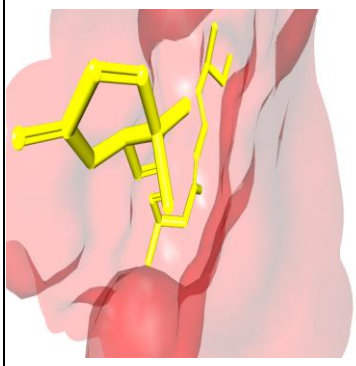
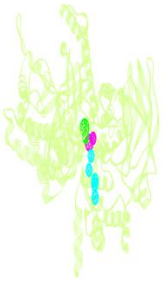
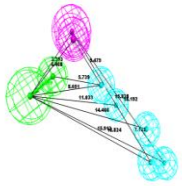
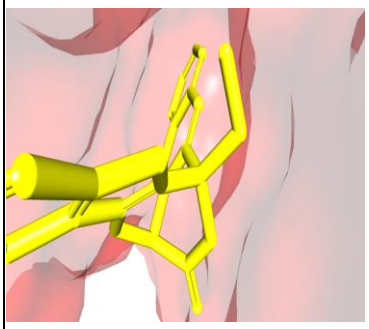
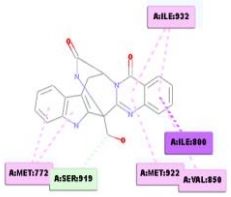
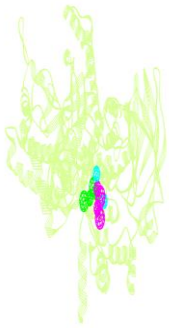
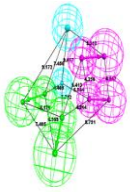
CMNPD22236 			
CMNPD25904 			
CMNPD26113 			
CMNPD26114 			

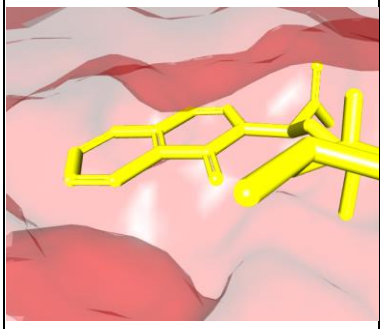
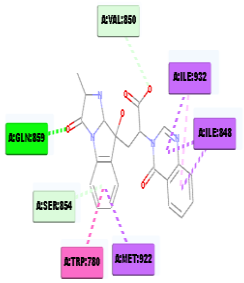
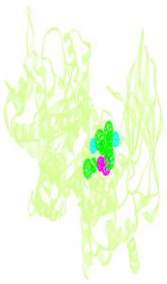
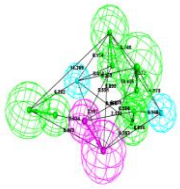
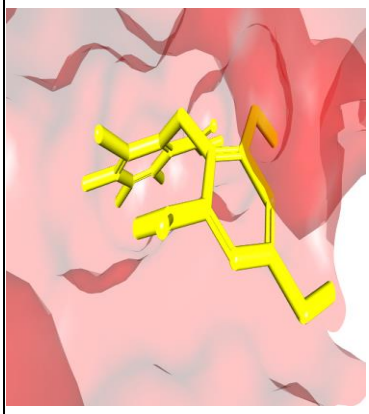
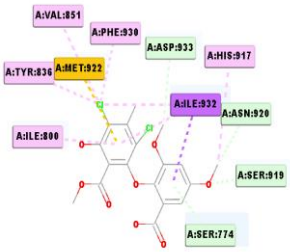
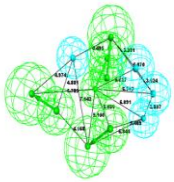
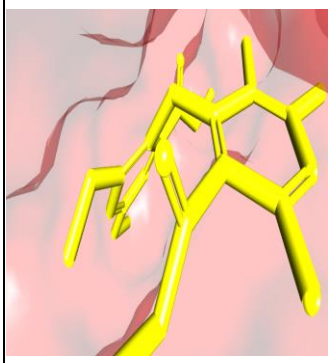
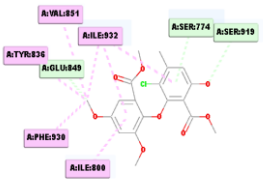
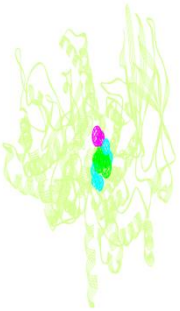
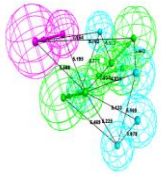
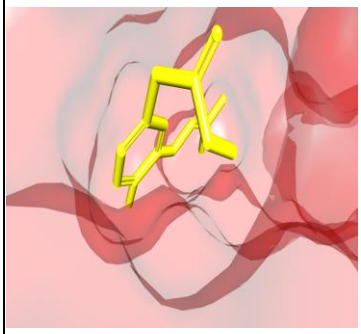
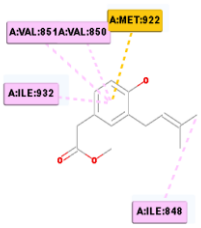
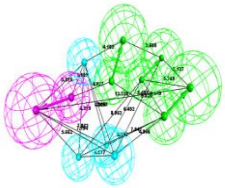
CMNPD28880 			
CMNPD28881 			
CMNPD28882 			
CMNPD28883 			

CMNPD28884 			
CMNPD28885 			
CMNPD28886 			
CMNPD28902 			

CMNPD28903 			
CMNPD28904 			
CMNPD28906 			
CMNPD28931 			

CMNPD28932 			
CMNPD28933 			
CMNPD28934 			
CMNPD28966 			

CMNPD29067 			
CMNPD29068 			
CMNPD29070 			
CMNPD30304 			

CMNPD30305 			
CMNPD30637 			
CMNPD30689 			
CMNPD30643 			

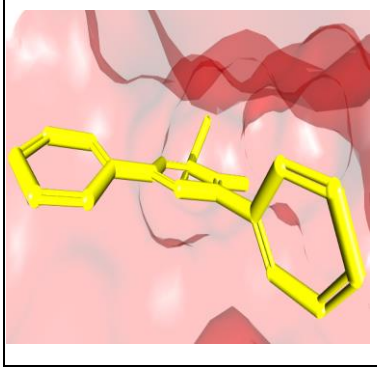
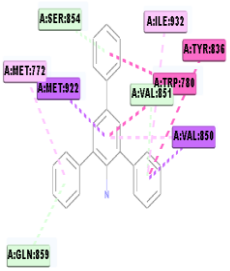
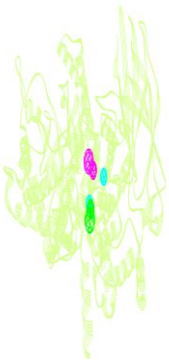
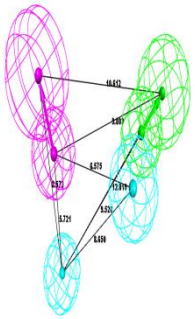
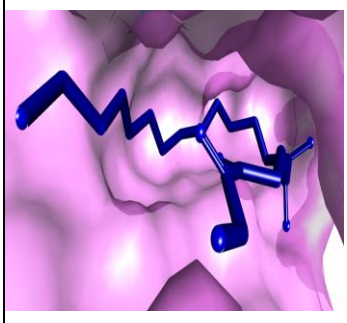
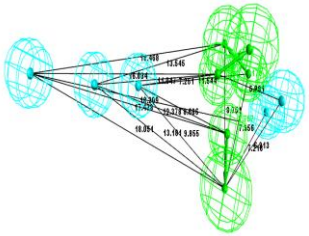
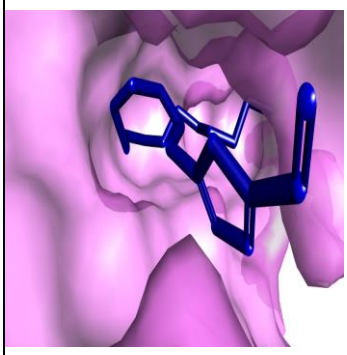
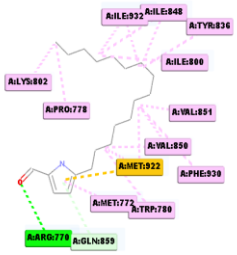
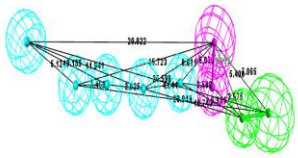
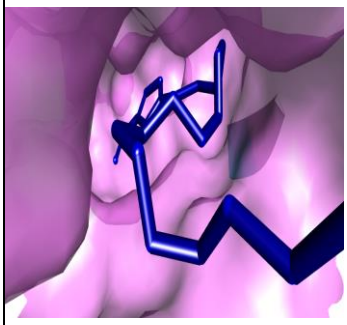
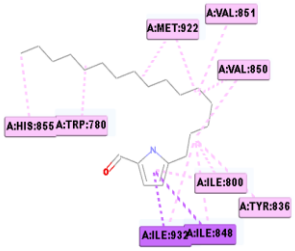
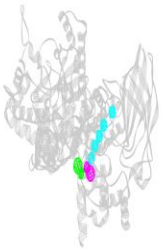
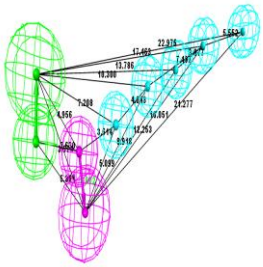
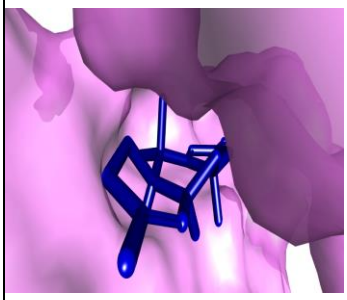
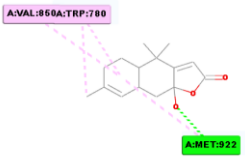
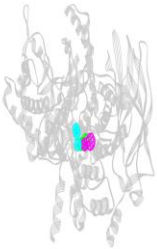
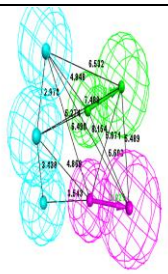
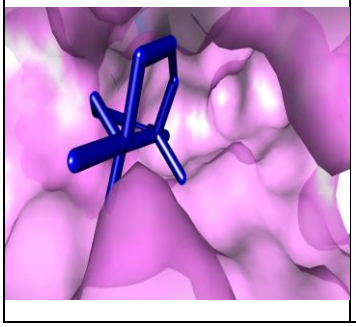
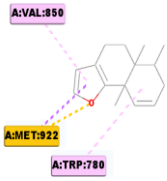
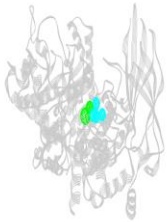
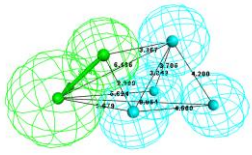
30821 			

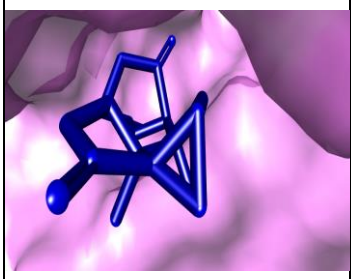
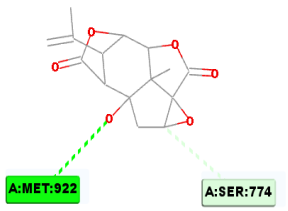
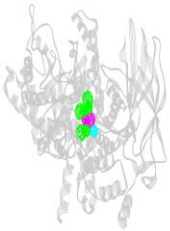
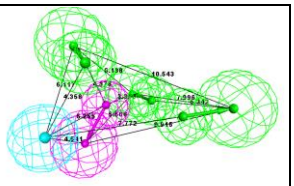
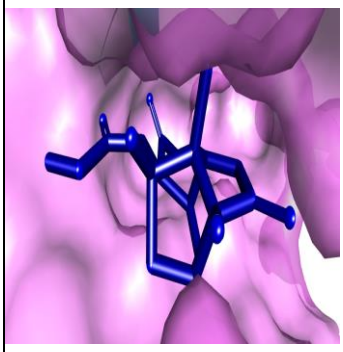
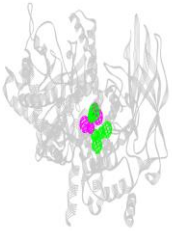
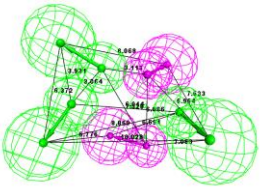
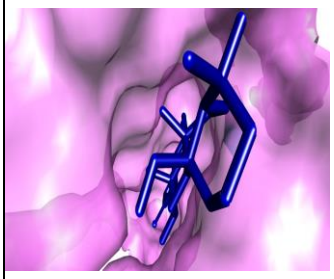
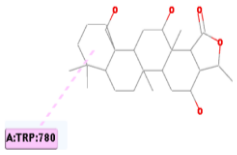
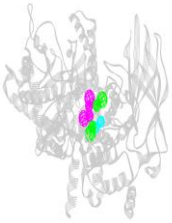
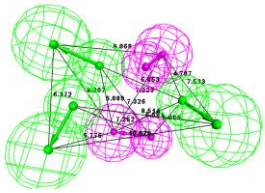
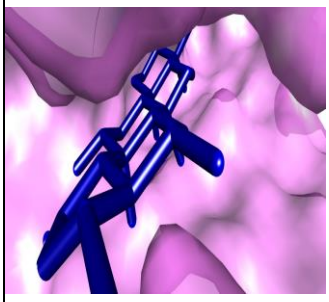
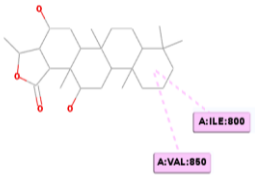
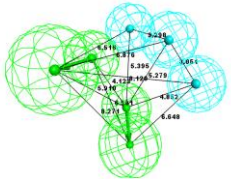
FIGURE 5.1.2

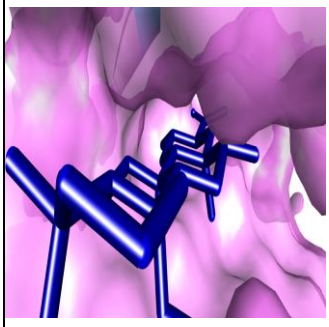
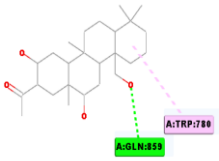
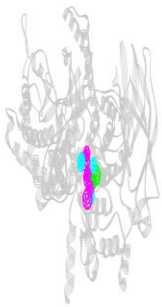
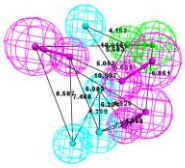
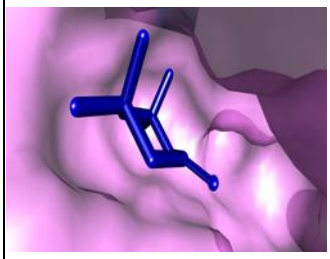
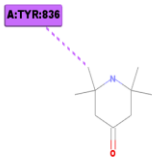
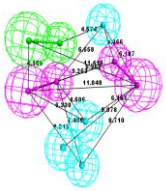
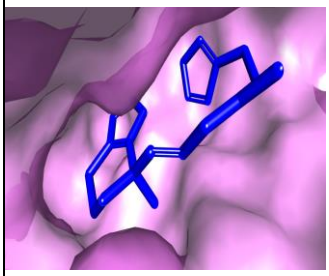
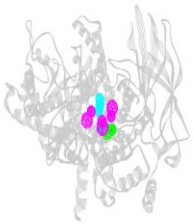
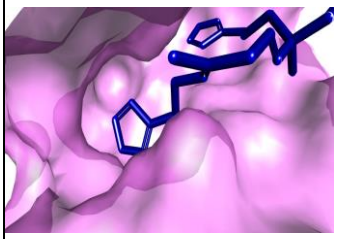
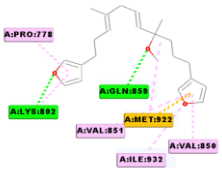
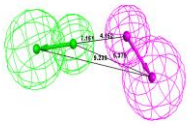
This table contains surface name, 2d structure, pharmacophore, geometry distance and structure (ligand interaction) Molecular docking of ligand and target. This figure indicates 3D and 2D interaction between target proteins a Triparanol interaction with 11βHSD.The pharmacophore features colors coded as cyan hydrophobic (HY), orange ring aromatic (RA) green hydrogen bond acceptor (HBA)**.**

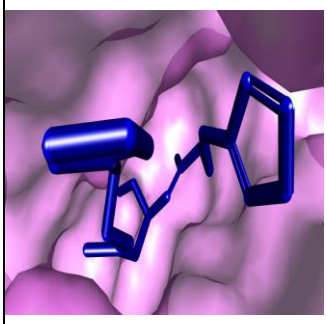
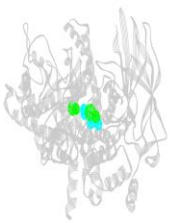
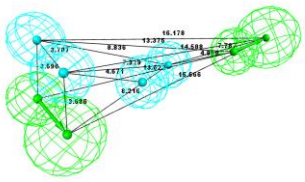
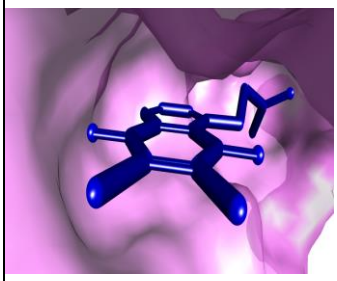
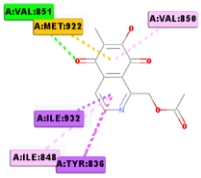
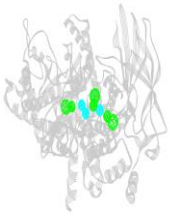
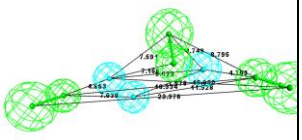
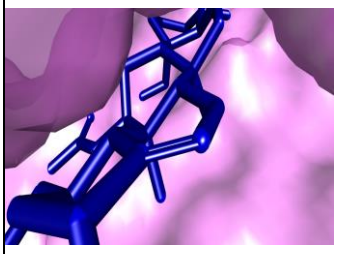
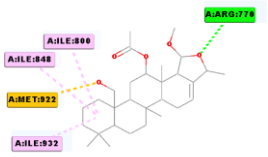
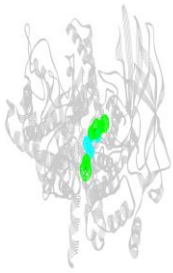
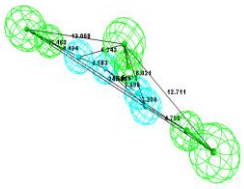
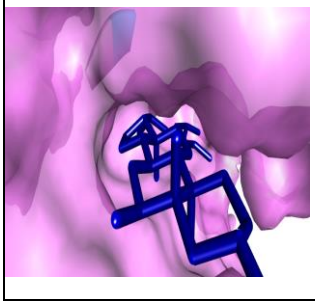
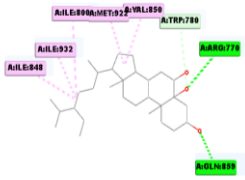
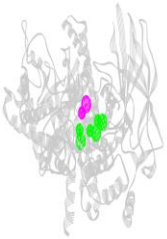
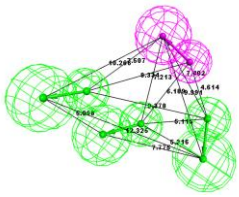
TABLE 5.6 2D ,3D STRUCTURE , PHARMACOPHORE AND GEOMETRY FOR MARINE SPONGES

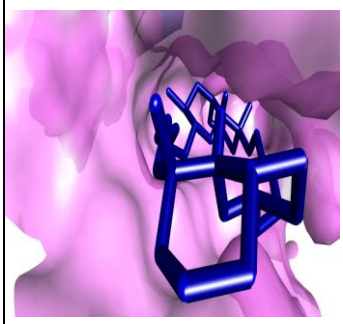
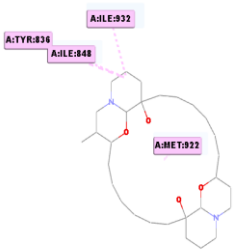
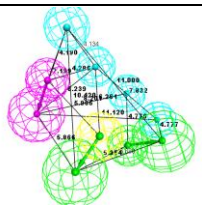
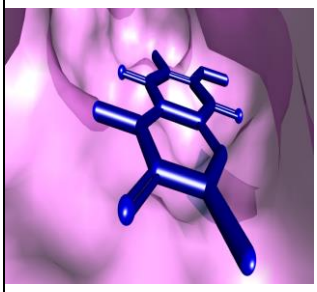
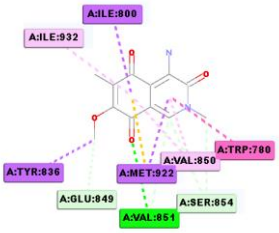
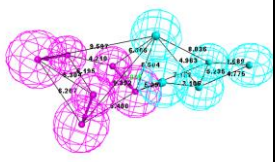
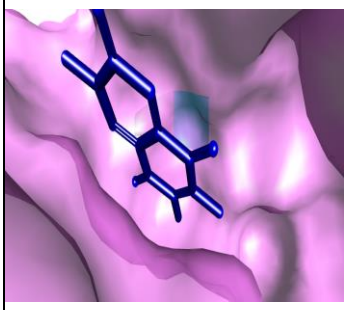
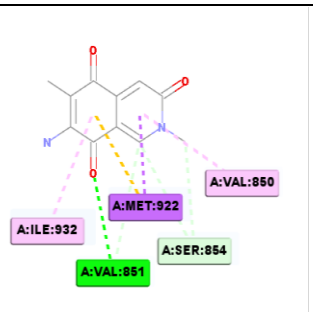
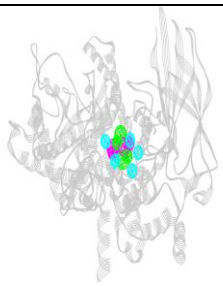
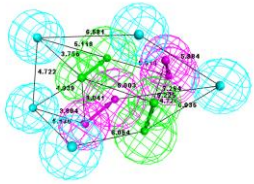
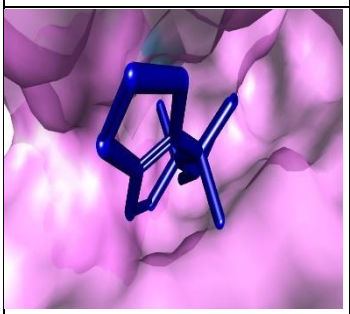
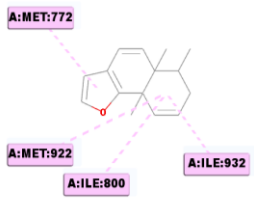
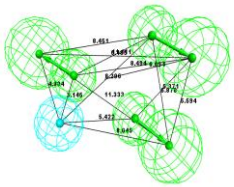
CMNPD878 			

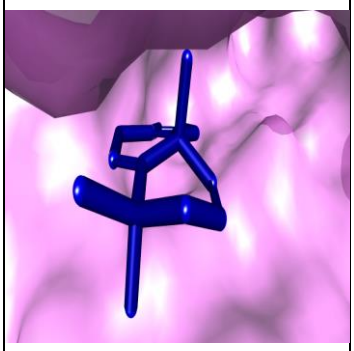
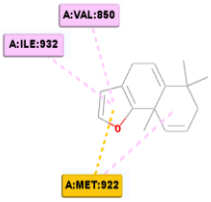
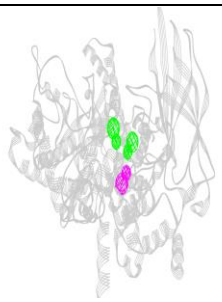
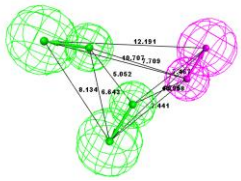
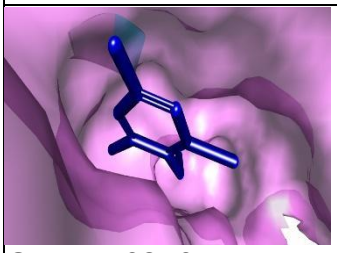
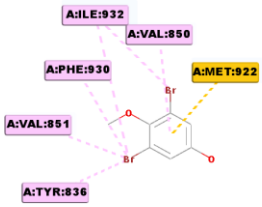
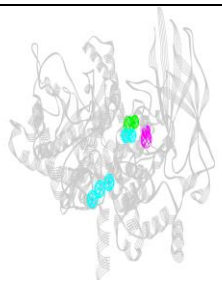
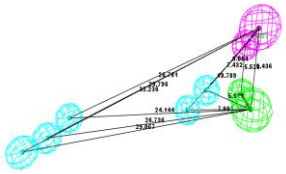
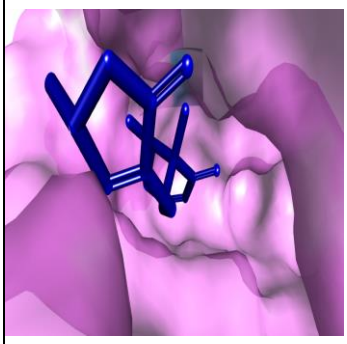
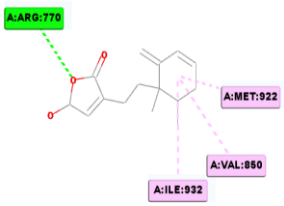
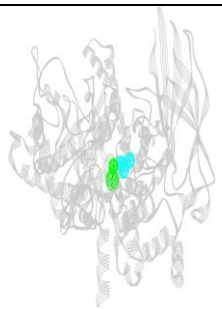
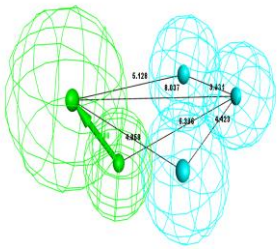
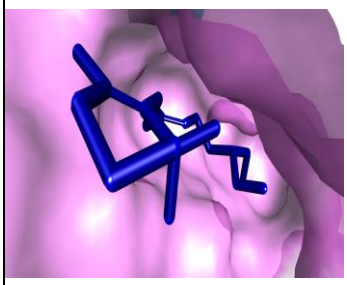
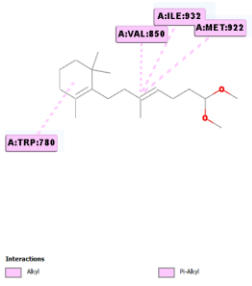
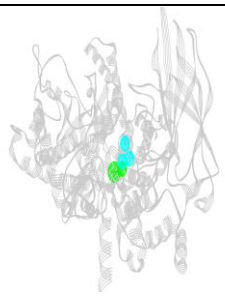
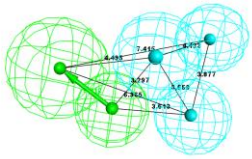
CMNPD966 			
CMNPD967 			
CMNPD1065 			
CMNPD2796 			

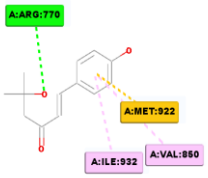
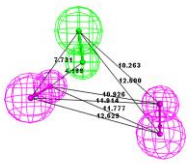
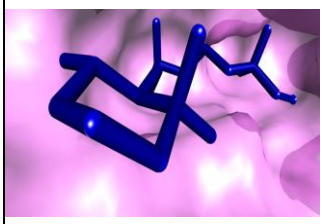
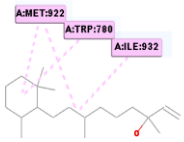
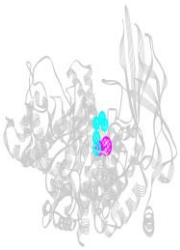
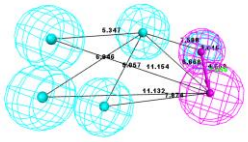
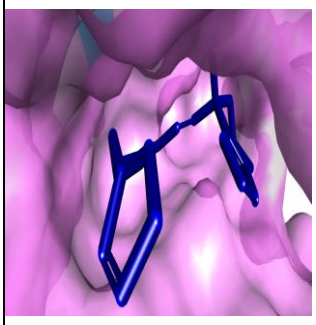
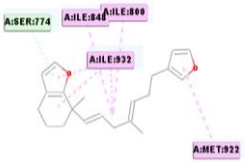
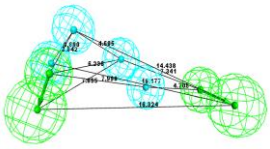
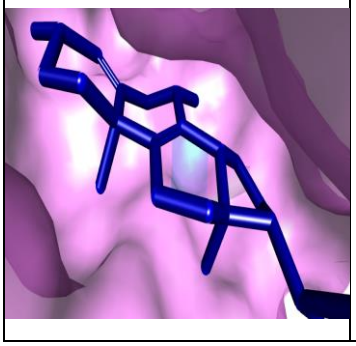
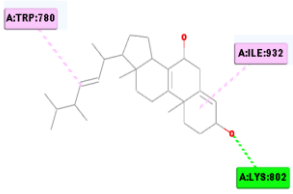
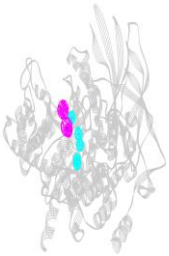
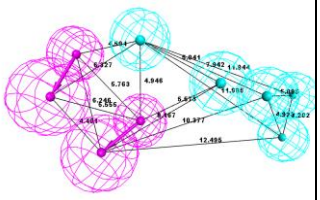
CMNPD2771 			
CMNPD2773 			
CMNPD5010 			
CMNPD5011 			

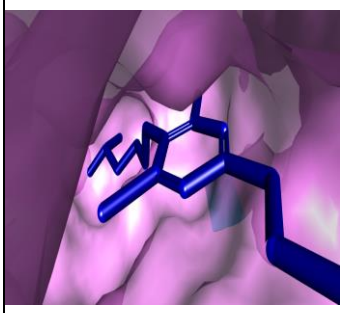
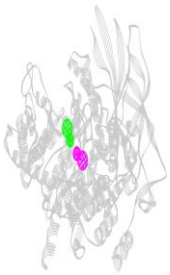
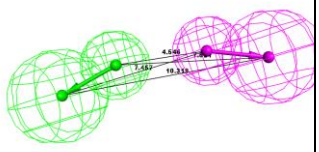
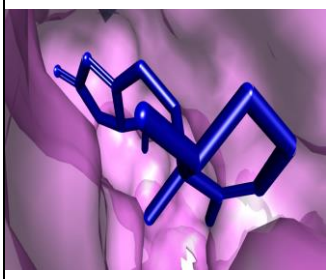
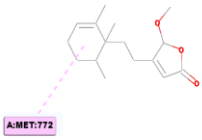
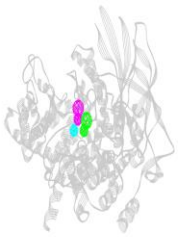
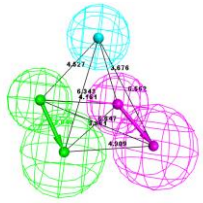
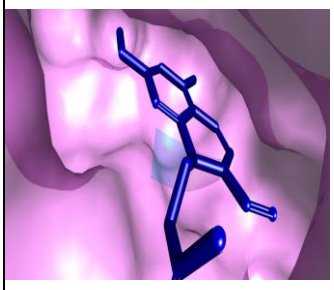
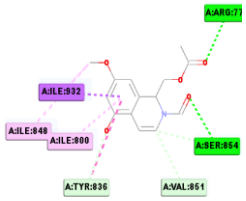
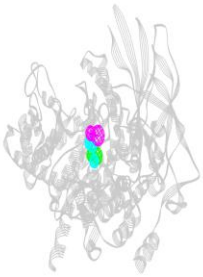
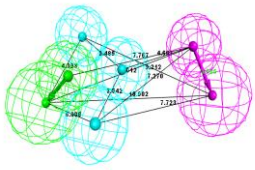
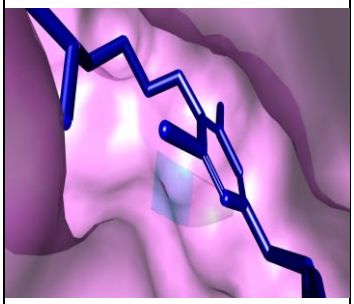
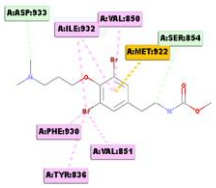
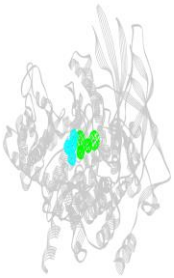
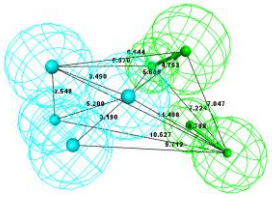
CMNPD5012 			
CMNPD5149 			
CMNPD5567 			
CMNPD5568 			

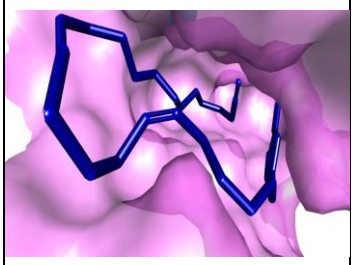
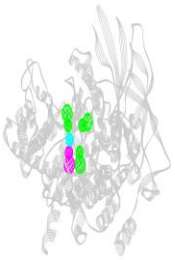
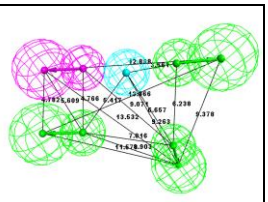
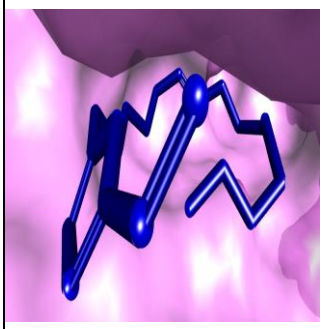
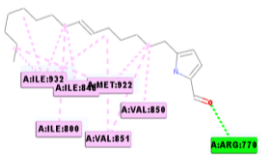
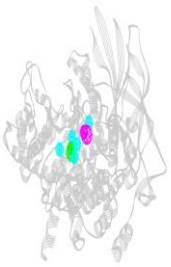
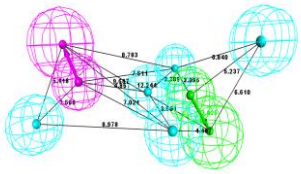
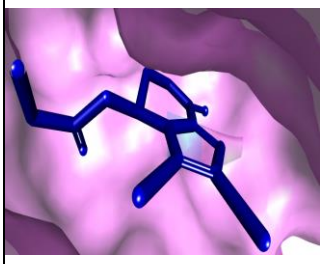
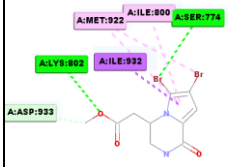
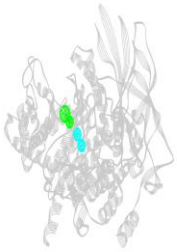
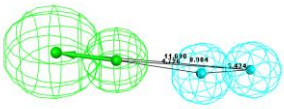
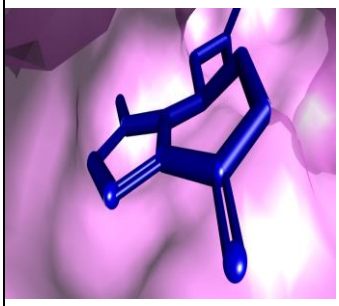
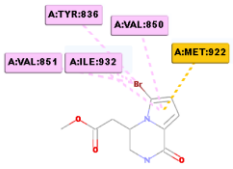
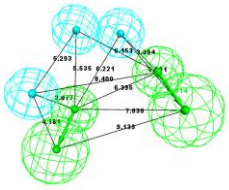
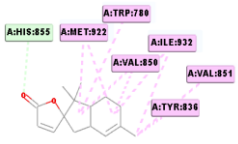
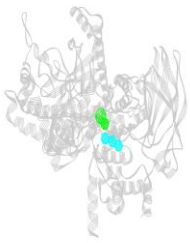
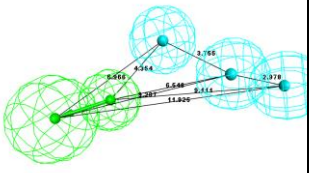
CMNPD5569 			
CMNPD6139 			
CMNPD6245 			
CMNPD6261 			

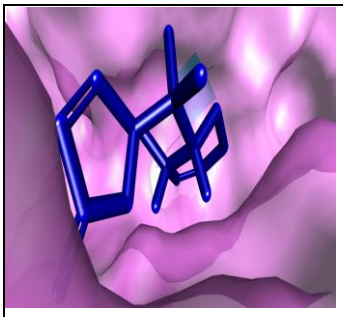
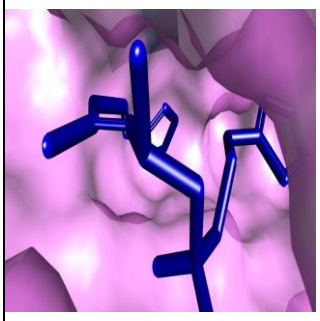
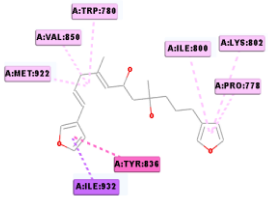
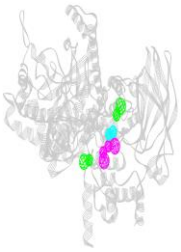
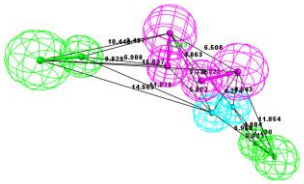
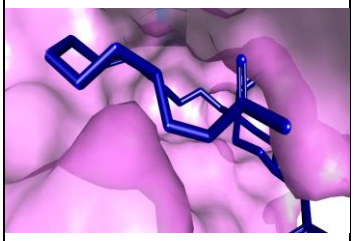
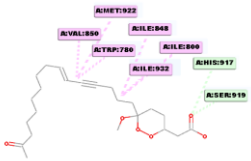
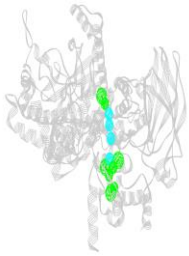
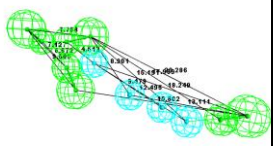
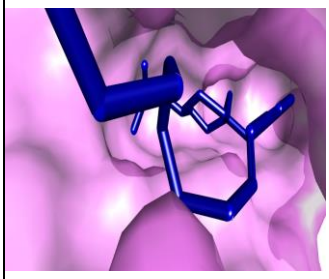
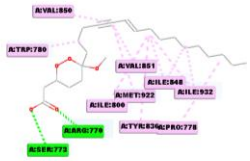
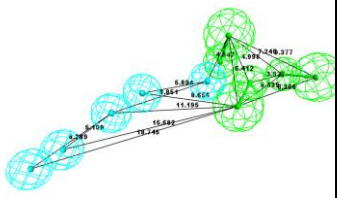
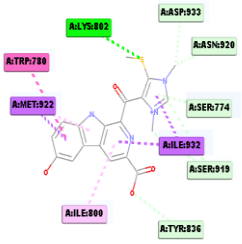
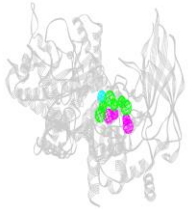
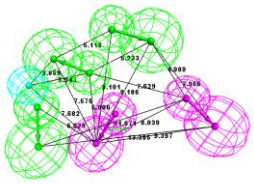
CMNPD6716 			
CMNPD6756 			
CMNPD6757 			
 CMNPD6874			

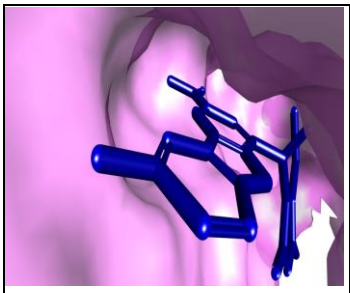
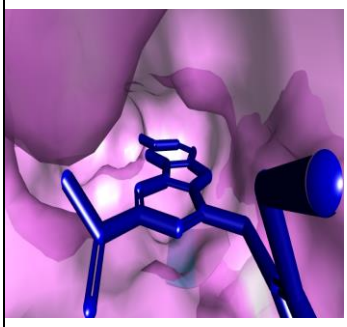
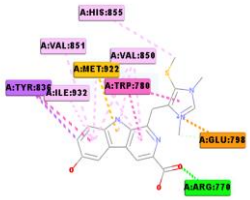
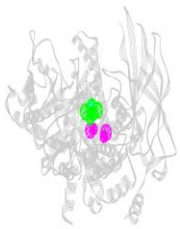
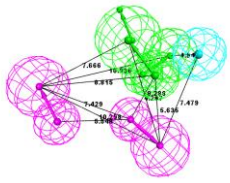
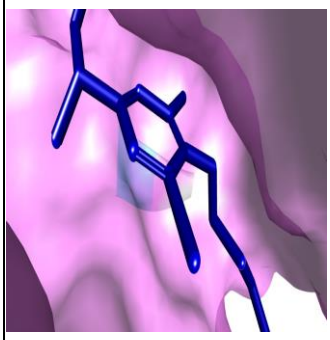
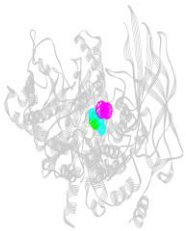
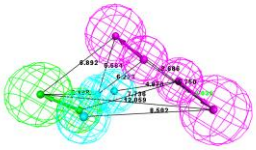
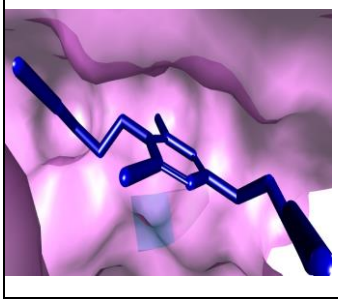
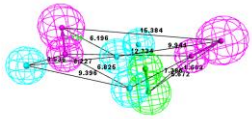
CMNPD6875 			
 CMNPD6876			
CMNPD6877 			
CMNPD6896 			

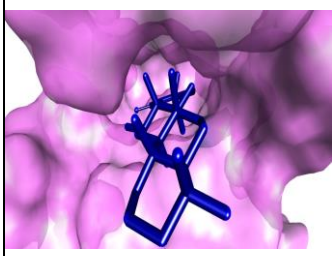
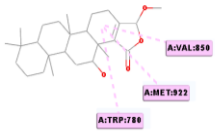
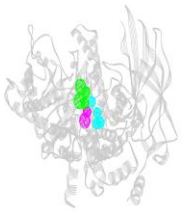
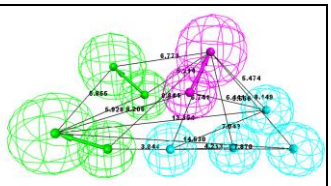
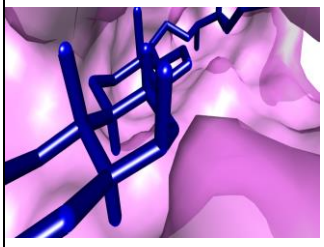
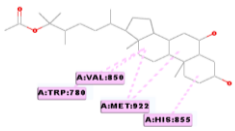
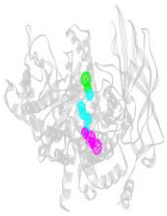
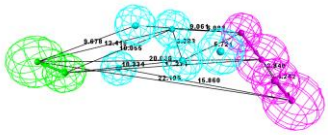
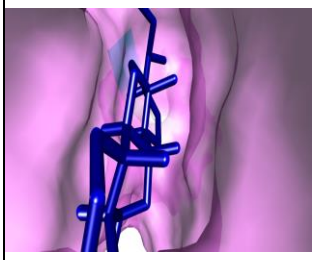
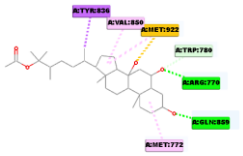
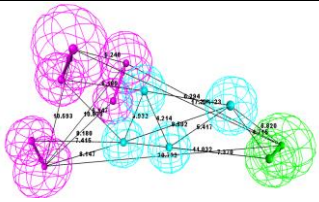
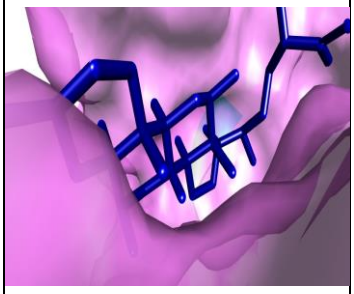
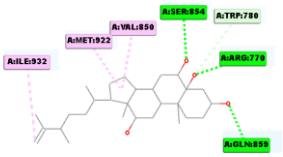
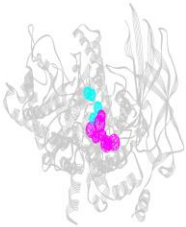
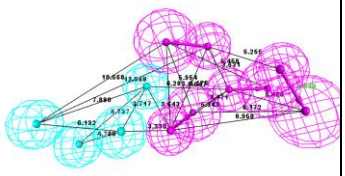
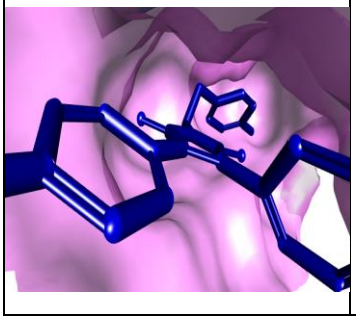
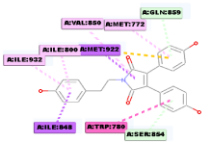
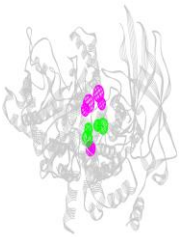
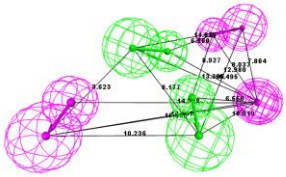
CMNPD7623 			
CMNPD7692 			
CMNPD8324 			
CMNPD8365 			

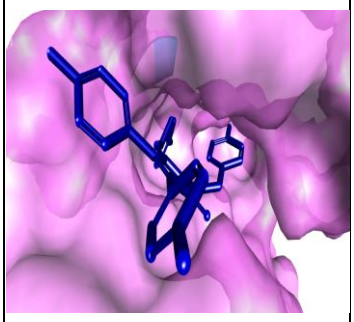
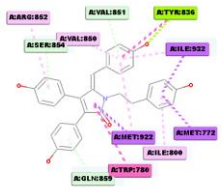
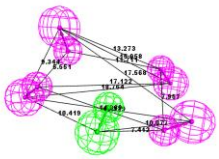
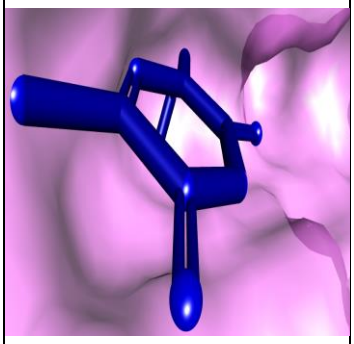
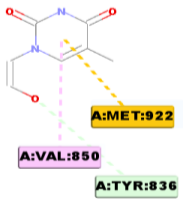
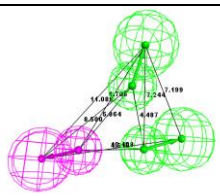
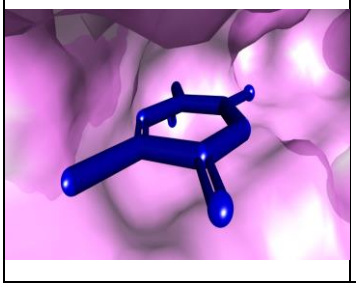
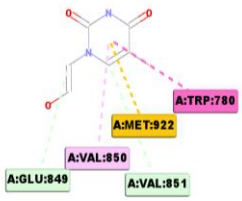
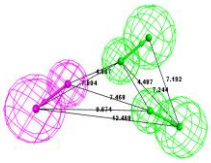
CMNPD9619 			
CMNPD9738 			
CMNPD10387 			
CMNPD10435 			

CMNPD11117 			
CMNPD11119 			
CMNPD11152 			
CMNPD11153 			
CMNPD11223			

			
CMNPD11249 			
CMNPD11843 			
CMNPD11844 			
CMNPD14212			

			
CMNPD14213 			
CMNPD14268 			
CMNPD15143 			

CMNPD18101 			
CMNPD20295 			
CMNPD20296 			
CMNPD20297 			
CMNPD25205 			

CMNPD25206 			
CMNPD25208 			
CMNPD25209 			

This table contains surface name, 2d structure, pharmacophore, geometry distance and structure (ligand interaction) Molecular docking of ligand and target. This figure indicates 3D and 2D interaction between target proteins a Triparanol interaction with 11βHSD.The pharmacophore features colors coded as cyan hydrophobic (HY), orange ring aromatic (RA) green hydrogen bond acceptor (HBA).

TABLE 5.7 TOPKAT RESULTS FOR MARINE BACTERIA

COMPOUND IDENTIFIER	Biodegradability	Test Ames: mutagen	FDA Mouse Female: Carcinogen	FDA Mouse Male: Carcinogen	RAT Female FD Carcinogen	RAT Male FD Carcinogen	Skin Irritancy	Skin Sensitizer	Predicted LD50
CMNPD30087	NO	YES	YES	YES	YES	YES	YES	NO	YES
CMNPD30086	NO	YES	YES	YES	YES	YES	YES	NO	YES
CMNPD29996	NO	NO	NO	YES	NO	NO	NO	NO	NO
CMNPD28614	NO	YES	YES	YES	YES	NO	NO	NO	YES
CMNPD28613	NO	NO	NO	NO	YES	NO	NO	NO	NO
CMNPD28608	NO	YES	NO	YES	YES	NO	NO	NO	NO
CMNPD28607	NO	YES	NO	YES	YES	NO	NO	NO	NO
CMNPD28606	NO	NO	NO	YES	YES	NO	NO	NO	NO
CMNPD28605	NO	NO	NO	YES	YES	NO	NO	NO	NO
CMNPD28508	NO	YES	NO	NO	YES	YES	NO	NO	NO
CMNPD28507	YES	NO	NO	YES	NO	YES	YES	NO	YES
CMNPD28506	NO	YES	NO	YES	YES	NO	YES	YES	YES
CMNPD25829	NO	YES	NO	NO	NO	NO	NO	NO	NO
CMNPD30117	YES	YES	YES	YES	NO	YES	YES	YES	NO
CMNPD27173	YES	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD27172	YES	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD27241	YES	YES	YES	YES	NO	YES	YES	YES	NO
CMNPD28694	NO	YES	NO	YES	NO	NO	NO	YES	YES
CMNPD24388	NO	YES	NO	YES	NO	NO	NO	NO	YES
CMNPD25827	YES	YES	NO	YES	NO	NO	YES	YES	YES
CMNPD30237	YES	YES	NO	YES	YES	YES	YES	YES	YES
CMNPD23280	NO	YES	NO	NO	NO	NO	NO	YES	NO
CMNPD21962	NO	YES	YES	NO	NO	YES	NO	NO	NO

CMNPD21961	NO	NO	YES	NO	NO	YES	NO	NO	NO
CMNPD21959	NO	NO	YES	NO	NO	YES	NO	NO	NO
CMNPD14698	NO	YES	YES	YES	NO	NO	YES	NO	NO

TABLE 5.8 TOPKAT RESULTS FOR MARINE FUNGI

COMPOUND IDENTIFIER	**Biodegradability**	**Test mes: mutagen**	**FD Mouse Female: Carcinogen**	**FD Mouse Mle: Carcinogen**	**RT Femle FD: Carcinogen**	**RT Mle FD: Carcinogen**	**Skin Irritancy**	**Skin Sensitizer**	**Predicted LD50**
CMNPD22236	NO	NO	NO	YES	YES	NO	NO	YES	NO
CMNPD15724	NO	NO	YES	YES	NO	NO	NO	NO	NO
CMNPD15725	NO	NO	YES	YES	NO	NO	NO	NO	NO
CMNPD12450	NO	NO	NO	YES	NO	NO	NO	NO	YES
CMNPD12451	NO	NO	NO	YES	NO	NO	NO	NO	YES
CMNPD30821	YES	YES	NO	NO	YES	YES	YES	YES	YES
CMNPD18724	NO	YES	NO	NO	NO	NO	YES	NO	NO
CMNPD18725	NO	YES	NO	YES	NO	NO	YES	YES	YES

CMNPD28911	NO	YES	NO	YES	NO	NO	NO	NO	YES
CMNPD25904	NO	YES	YES	YES	NO	YES	NO	NO	YES
CMNPD26113	NO	YES	YES	YES	NO	NO	NO	NO	NO
CMNPD26114	NO	YES	YES	YES	YES	YES	YES	NO	YES
CMNPD28880	NO	NO	YES	YES	NO	YES	YES	YES	YES
CMNPD28881	YES	NO	YES	YES	NO	YES	NO	YES	YES
CMNPD28882	YES	YES	YES	YES	NO	YES	NO	YES	YES
CMNPD28883	YES	NO	YES	YES	YES	YES	NO	YES	YES
CMNPD28884	NO	NO	YES	YES	NO	YES	NO	YES	YES
CMNPD28885	YES	NO	YES	YES	NO	YES	YES	YES	YES
CMNPD28886	YES	NO	YES	YES	NO	YES	YES	YES	YES
CMNPD28902	NO	YES	NO	YES	NO	NO	NO	NO	NO
CMNPD28903	NO	NO	NO	NO	NO	NO	YES	NO	YES
CMNPD28904	NO	NO	NO	NO	NO	YES	NO	NO	NO
CMNPD28906	NO	YES	YES	YES	YES	YES	YES	NO	YES
CMNPD28931	NO	YES	YES	YES	YES	YES	NO	YES	YES
CMNPD28932	NO	YES	YES	YES	YES	YES	NO	YES	YES
CMNPD28933	YES	YES	YES	YES	YES	YES	NO	NO	YES
CMNPD28934	YES	YES	YES	YES	YES	YES	NO	NO	YES
CMNPD28965	YES	YES	YES	YES	NO	YES	YES	YES	YES
CMNPD28966	NO	YES	YES	YES	YES	YES	YES	YES	NO
CMNPD29067	NO	YES	NO	NO	YES	NO	NO	NO	NO
CMNPD29068	NO	YES	NO	NO	YES	NO	NO	NO	NO
CMNPD29070	NO	YES	NO	YES	YES	NO	NO	NO	NO
CMNPD30304	NO	YES	NO	NO	NO	NO	NO	NO	NO
CMNPD30305	NO	NO	YES	YES	NO	NO	NO	NO	NO

CMNPD30637	NO	YES	YES	YES	YES	YES	NO	NO	YES
CMNPD30638	NO	YES	YES	YES	YES	YES	NO	NO	YES
CMNPD30639	NO	YES	YES	YES	YES	YES	NO	NO	YES
CMNPD30643	NO	NO	NO	YES	YES	YES	YES	YES	NO
CMNPD21959	NO	NO	YES	NO	NO	YES	NO	NO	YES
CMNPD14698	NO	YES	YES	YES	NO	NO	YES	NO	NO

TABLE 5.9 TOPKAT RESULTS FOR MARINE SPONGES

COMPOUND IDENTIFIER	**Biodegradability**	**Testmes: mutagen**	**FD Mouse Female: Carcinogen**	**FD Mouse Mle: Carcinogen**	**RT Female FDA Carcinogen**	**RT Mle FDA Carcinogen**	**Skin Irritancy**	**Skin Sensitizer**	**Predicted LD50**
CMNPD5567	NO	NO	NO	YES	YES	NO	NO	NO	NO
CMNPD5568	NO	NO	NO	NO	YES	NO	NO	NO	NO
CMNPD5569	NO	NO	NO	NO	YES	NO	NO	NO	NO
CMNPD8981	YES	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD8982	YES	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD878	YES	NO	NO	YES	YES	NO	NO	YES	YES
CMNPD966	NO	YES	NO	YES	NO	NO	YES	YES	NO
CMNPD967	NO	YES	NO	YES	NO	NO	YES	YES	NO
CMNPD2769	NO	NO	NO	NO	NO	NO	NO	NO	NO
CMNPD2771	YES	NO	NO	YES	YES	NO	NO	NO	NO

CMNPD2772	NO	NO	NO	YES	YES	NO	NO	NO	NO
CMNPD2773	NO	YES	NO	NO	YES	NO	NO	NO	NO
CMNPD5149	NO	YES	NO	NO	YES	NO	YES	YES	YES
CMNPD6139	NO	NO	NO	YES	YES	YES	YES	YES	YES
CMNPD6245	NO	NO	NO	YES	NO	NO	NO	YES	NO
CMNPD6261	NO	YES	NO	NO	YES	NO	NO	NO	YES
CMNPD6756	NO	NO	NO	YES	YES	YES	YES	NO	YES
CMNPD6757	YES	YES	NO	YES	YES	YES	YES	YES	YES
CMNPD6872	NO	NO	NO	NO	YES	NO	NO	NO	NO
CMNPD7692	NO	YES	NO	YES	YES	NO	YES	NO	YES
CMNPD14212	NO	YES	YES	YES	YES	YES	NO	YES	YES
CMNPD14213	NO	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD9619	NO	YES	YES	YES	NO	YES	YES	NO	YES
CMNPD10387	YES	YES	NO	YES	YES	YES	NO	YES	YES
CMNPD10435	NO	YES	YES	YES	NO	YES	NO	NO	YES
CMNPD11152	NO	YES	YES	YES	NO	NO	NO	NO	YES
CMNPD11223	NO	YES	NO	YES	NO	NO	YES	YES	YES
CMNPD25205	YES	YES	NO	YES	YES	YES	YES	YES	YES
CMNPD25206	NO	NO	NO	YES	YES	NO	NO	NO	YES
CMNPD25208	NO	YES	NO	YES	YES	YES	YES	YES	YES
CMNPD25209	NO	YES	NO	YES	YES	YES	YES	YES	YES
CMNPD9738	YES	YES	NO	YES	YES	NO	NO	NO	YES
CMNPD20295	NO	YES	YES	NO	YES	NO	NO	YES	YES
CMNPD20297	NO	NO	NO	NO	YES	NO	NO	YES	YES
CMNPD5010	NO	NO	NO	NO	YES	NO	NO	NO	YES
CMNPD5011	NO	NO	NO	NO	YES	NO	NO	YES	YES
CMNPD5012	NO	YES	NO	YES	YES	NO	YES	YES	YES
CMNPD6874	NO	NO	NO	YES	YES	NO	NO	YES	NO

CMNPD6875	NO	NO	NO	YES	YES	NO	NO	NO	YES
CMNPD6876	YES	YES	YES	YES	NO	YES	YES	YES	YES
CMNPD6716	NO	YES	NO	YES	YES	NO	NO	NO	YES
CMNPD6877	YES	YES	NO	YES	YES	NO	NO	YES	YES
CMNPD6896	NO	NO	NO	NO	YES	NO	NO	NO	NO
CMNPD8324	NO	NO	NO	YES	YES	NO	NO	NO	NO
CMNPD11249	NO	YES	NO	YES	YES	NO	NO	NO	NO
CMNPD11843	NO	YES	NO	YES	YES	YES	NO	YES	YES
CMNPD11844	NO	YES	NO	YES	YES	NO	NO	YES	NO
CMNPD11117	NO	NO	NO	NO	NO	NO	NO	YES	NO
CMNPD11118	NO	NO	NO	YES	NO	NO	NO	YES	NO
CMNPD11119	NO	YES	NO	YES	NO	NO	NO	YES	NO
CMNPD18101	NO	NO	NO	NO	YES	NO	NO	YES	NO
CMNPD20296	NO	YES	NO	YES	YES	NO	NO	YES	YES
CMNPD11153	NO	YES	YES	YES	YES	NO	YES	YES	YES
CMNPD7623	YES	NO	YES	YES	YES	YES	YES	YES	YES
CMNPD1065	YES	YES	NO	YES	YES	YES	NO	YES	NO
CMNPD3038	NO	YES	NO	YES	YES	YES	NO	YES	NO
CMNPD15143	NO	YES	YES	YES	NO	YES	NO	NO	YES
CMNPD10459	YES	YES	YES	YES	YES	YES	YES	YES	YES
CMNPD14268	NO	YES	YES	YES	NO	YES	YES	NO	YES
CMNPD8365	NO	NO	NO	NO	NO	NO	NO	YES	NO

Top Kat (Toxicity Prediction by Komputer Assisted Technology) This life science application supports in silico target characterization and lead optimization using a wealth of trusted life science modeling and simulation methods. This quantifies electronic, bulk and shape attributes of a structure in terms of electro topological state (E-states) values of all possible two-atom fragment, atomic size adjusted E-states computed from rescaled

count of valence electrons, molecular weight, topological shape indices, and symmetry indices. The methodology is an extension of classic quantitative structure–activity relationships (QSAR).

TABLE 5.10 DOCK SCORE TABLE FOR MARINE BACTERIA

COMPOUND IDENTIFIER	Lig Score1_Dreiding	Lig Score2_Dreiding	-PLP 1	-PLP 2	JAIN	DOCK SCORE
CMNPD21962	4.92	6.18	87.17	65.08	0.66	73.768
CMNPD21959	3.24	5.41	67.71	63.73	-0.73	67.156
CMNPD28606	3.93	6.21	91.17	91.17	-1.41	66.593
CMNPD28607	3.48	5.5	67.39	56.09	-1.01	63.44
CMNPD21961	3.72	5.46	68.18	68.19	-0.18	60.556
CMNPD28605	2.25	4.64	79.59	73.06	-1.35	59.781
CMNPD28614	2.9	5.18	78.73	69.7	-0.68	58.859
CMNPD30087	3.83	5.56	49.54	47.83	-2.4	57.329
CMNPD21959	4.19	5.12	66.31	67.19	0.17	56.01
CMNPD14698	2.74	5.4	70.76	50.24	-2.31	54.012
CMNPD28508	2.81	4.52	51.7	54.24	-1.46	54.002
CMNPD27172	2.71	4.85	55.94	49.97	-0.77	53.762
CMNPD28608	1.85	4.83	71.87	68.25	-0.27	53.193
CMNPD28613	1.66	4.48	76.06	74.31	0.29	53.179
CMNPD28506	3.5	5.69	66.92	60.15	-1.39	52.709
CMNPD25827	2.13	5.13	63.68	63.72	-1.18	51.384
CMNPD27173	1.74	4.24	52.38	47.03	-1.22	49.207
CMNPD30117	2.76	4.7	52.52	47.72	-1.81	48.728
CMNPD27241	2.76	4.7	52.52	47.72	-1.81	45.752
CMNPD28507	2.91	5.03	66.13	67.38	-0.02	44.669
CMNPD30086	1.68	4.32	67.64	64.84	-0.39	43.233
CMNPD30237	1.05	3.72	43.34	37.32	-0.52	43.233

CMNPD25829	2.35	3.47	60.99	62.39	-1.16	42.219

TABLE 5.11 DOCK SCORE TABLE FOR MARINE FUNGI

Compound Identifier	Lig Score1_ Dreiding	Lig Score2_ Dreiding	-PLP 1	-PLP 2	JAIN	-PMF	DOCK SCORE
CMNPD28906	5.68	6.03	79.73	65.63	-2.35	74.01	77.652
CMNPD30305	2.84	5.99	91.78	79.8	-1.18	75.92	77.365
CMNPD30639	4.25	6.22	74.8	66.23	-2.42	55.31	76.902
CMNPD30637	5.36	5.96	80.04	63.57	-2.11	53.62	75.084
CMNPD30638	4.1	5.82	80.03	66.77	-2.8	61.02	74.953
CMNPD28902	6.88	6.62	70.35	42.98	-2.53	103.45	74.069
CMNPD29068	6.11	6.83	68.95	61.4	-3.27	87.72	70.675
CMNPD29067	4.61	6.11	77.37	71.23	-2.96	73.3	70.19
CMNPD29070	3.64	6.29	67.31	58.75	-3.23	85.05	68.603
CMNPD28904	4	6.2	76.54	69.87	-1.78	108.07	67.692
CMNPD21959	3.24	5.41	67.71	63.73	-0.73	34.85	67.156
CMNPD28903	4.61	5.29	70.46	59.98	-1.45	129.83	66.226
CMNPD28966	3.92	5.63	74.5	60.03	-1.2	72.08	56.751
CMNPD28965	3.57	5.35	70.17	58.61	-1.81	80.91	56.131
CMNPD28932	4.06	5.32	65.56	57.93	-0.98	64.62	55.432
CMNPD14698	2.74	5.4	70.76	50.24	-2.31	77.26	54.012

CMNPD30643	2.7	5.18	65.16	57.46	-2.26	74.05	53.922
CMNPD28934	3.15	5.24	64.5	50.51	-1.14	67.76	53.617
CMNPD28933	3.38	5.22	56.78	49.48	-1.35	57.9	52.986
CMNPD28931	3.12	5.45	65.58	52.15	-2.24	73.03	51.582
CMNPD28886	3.35	4.69	49.57	39.84	-2.63	59.81	47.066
CMNPD30304	2.67	4.25	49.51	38.75	0.01	21.19	44.868

TABLE 5.12 DOCK SCORE TABLE FOR MARINE SPONGES

Compound Identifier	Lig Score1_ Dreiding	Lig Score2_ Dreiding	-PLP 1	-PLP 2	JAIN	-PMF	DOCK SCORE
CMNPD6261	3.93	6.95	86.64	85.01	-2.04	133.95	86.322
CMNPD8365	4.38	7.38	86.61	79.46	-2.43	100.81	82.129
CMNPD25206	2.94	6.54	109.06	100.76	-0.74	89.45	82.005
CMNPD14213	3.82	5.9	86.07	72.06	-1.94	82.66	79.531
CMNPD11118	3.71	6.53	82.1	75.07	-3.19	74.86	76.65
CMNPD5569	3.96	6.15	70.41	62.45	-3.41	64.74	76.109
CMNPD5568	4.83	5.86	57.42	54.71	-3.46	63.4	75.653
CMNPD14212	5.99	6	66.34	55.25	-1.73	53.32	75.401
CMNPD20295	2.68	6.3	82.39	78.6	-2.28	101.41	75.223
CMNPD11843	4.69	6.12	73.47	57.08	-3.99	50.83	74.886
CMNPD11249	3.8	6.45	77.29	72.32	-3.38	73.04	74.675
CMNPD967	2.73	6.23	79.59	73.78	-3.73	76.61	74.509
CMNPD11844	4.36	6.13	77.37	68.1	-3	72.96	74.092
CMNPD11119	3.84	6.35	57.95	61.27	-3.49	79	73.533
CMNPD20297	3.8	6.37	80.24	77.04	-1.74	121.39	72.821
CMNPD878	4.48	6.29	73.17	63.59	-3.89	68.52	71.992
CMNPD966	3.68	6.57	69.63	63.7	-3.49	60.82	71.904
CMNPD5567	3.62	6.23	87.98	83.78	-1.61	91.15	70.178
CMNPD8324	2.98	5.81	66.81	64.56	-1.78	75.37	69.692
CMNPD20296	3.76	5.95	75.28	73.1	-2.75	105.58	69.689
CMNPD25205	3.59	6.88	91.56	68.88	-1.51	93.66	68.492

CMNPD6896	2.7	5.87	70.11	67.24	-3.29	84.6	66.565
CMNPD7692	2.29	5.72	63.54	61.6	-3.25	69.8	65.448
CMNPD10435	3.13	6.05	77.53	62.04	-2.71	71.19	65.272
CMNPD15143	2.97	5.79	75.12	57.99	-2.26	68.26	64.361
CMNPD6245	4.23	5.54	51.41	46.96	-2.19	88.26	64.289
CMNPD11117	2.52	4.96	59.72	72.15	-4.02	40.17	63.171
CMNPD5010	2.34	5.21	59.77	53.86	-1.91	87.78	60.096
CMNPD9619	2.27	5.46	71.73	61.56	-2.21	46.04	59.936
CMNPD10387	3.8	5.54	68.42	58.4	-1.93	80.36	58.305
CMNPD14268	2.44	5.16	64.26	54.68	-2.87	44.79	57.737
CMNPD5012	2.02	5.03	53	50.56	-2.75	95.78	56.049
CMNPD6716	1.4	3.41	44.35	48.42	-0.04	62.94	54.683
CMNPD6139	2.52	5.29	66.53	59.62	-1.78	78.76	53.006
CMNPD11152	3.31	4.7	46.36	37.95	-2.21	35.96	50.506
CMNPD18101	1.58	4.29	45.87	47.65	-1.87	93.09	49.209
CMNPD7623	3.05	5.13	53.2	45.86	-2.36	73.34	48.776
CMNPD2772	2.84	4.3	40.74	28.94	-1.91	34.7	48.464
CMNPD9738	2.63	4.72	52.93	48.01	-2.35	55.09	48.367
CMNPD11153	2.92	4.8	55.65	49.66	-1.32	47.67	48.114
CMNPD6877	2.8	4.83	45.13	36.21	-2.12	76.8	46.216
CMNPD2773	4.42	4.38	46.05	23.88	-1.83	53.63	43.916
CMNPD6756	4.01	4.8	62.21	44.6	-1.72	64.6	43.315
CMNPD5011	1.42	4.16	57.78	48.8	-1.79	91.35	42.99
CMNPD6875	1.85	4.37	50.66	46.38	-1.36	48.46	42.691
CMNPD6757	3.01	4.65	58.01	43.23	-1.18	60.58	42.624
CMNPD1065	1.62	4.61	56.86	53.16	-0.97	56.5	42.356
CMNPD2771	2.69	4.21	38.43	25.06	-1.38	30.87	41.713
CMNPD3038	2.79	3.73	25.66	29.91	-2.05	58.22	37.237
CMNPD11223	1.64	4.04	44.67	36.61	-1.32	57.65	35.621
CMNPD2769	1.76	3.63	36.65	35.83	-1.05	45.95	35.102
CMNPD6876	1.22	3.92	43.48	38.91	-1.54	27.43	35.022
CMNPD10459	2.68	3.78	44.94	37.82	-1.37	40.54	34.758
CMNPD25208	1.92	4.37	47.2	37.89	-1.47	30.03	34.155
CMNPD6874	1.02	3.8	34.04	31.44	-1.31	55.56	34.071
CMNPD25209	1.8	4.17	49.05	39.29	-1.43	37	33.733
CMNPD5149	1.05	3.8	41.52	36.21	-1.33	24.18	31.071

CMNPD8982	1.55	3.56	39.12	33.5	-1.53	33.72	25.349
CMNPD8981	1.95	3.36	46.95	33.9	-1.06	21.01	23.849

DOCK SCORE

Dock Score is an objective scoring scheme that can be used to rank protein-protein docked poses. It considers several interface parameters, namely, surface area, evolutionary conservation, hydrophobicity, short contacts and spatial clustering at the interface for scoring. Dock Score to perform the ranking of the docked poses. It utilizes the parameters of the interface formed upon interaction of the given protein chains. These interface parameters are surface area, conserved residues, hydrophobicity, short contacts and spatial clustering. Dock Score webserver can be employed, subsequent to docking, to perform scoring of the docked solutions, starting from multiple poses as inputs

TABLE 5.13 MARINE BACTERIA DFT TABLE

COMPOUND IDENTIFIER	**HOMO ENERGY (EV)**	**LUMO ENERGY (EV)**	**BINDING GAP ENERGY (EV)**
CMNPD30087	-6.415817668	-1.598376624	4.817441044
CMNPD30086	-6.720059341	-1.467771161	5.25228818
CMNPD29996	-5.746423511	-1.668102841	4.07832067
CMNPD28614	-6.209706831	-1.526753229	4.682953602
CMNPD28613	-6.056798361	-1.558888259	4.497910103
CMNPD28608	-5.563089432	-0.4440111186	5.119078313
CMNPD28607	-5.943751325	-0.5340794887	5.409671836
CMNPD28606	-6.032195719	-0.4115778522	5.620617867
CMNPD28605	-5.988381557	-0.4579694779	5.530412079
CMNPD28508	-5.898415502	-0.6033822961	5.295033206
CMNPD28507	6.050139188 -	-1.119950161	4.930189026
CMNPD28506	-6.251152241	-1.492470948	4.758681293
CMNPD25829	-5.868635891	-1.395527618	4.473108273

CMNPD30117	7.366528166 -	-0.3736946867	6.992833479
CMNPD27173	-7.450574653	-2.032862665	5.417711988
CMNPD27172	-7.408882436	-2.002995161	5.405887275
CMNPD27241	-7.366528166	-0.3736946867	6.992833479

TABLE 5.14 MARINE FUNGI DFT TABLE

COMPOUND IDENTIFIER	**HOMO ENERGY (eV)**	**LUMO ENERGY (eV)**	**Binding gp energy (eV)**
CMNPD22236	-5.478998045	-1.312150803	4.166847243
CMNPD15724	-6.546055778	-1.908551742	4.637504036
CMNPD15725	-6.357612486	-1.968732473	4.388880013
CMNPD12450	-6.272638362	-2.494238194	3.778400168
CMNPD12451	-6.270140083	-2.489737973	3.780402111
CMNPD30821	-5.061713691	-0.945691083	4.116022608
CMNPD18724	-5.743609853	-2.219018839	3.524591014
CMNPD18725	-6.155149881	-2.166759619	3.988390262
CMNPD28911	-6.416578499	-2.89209497	3.524483529
CMNPD25904	-6.086669946	-2.427017875	3.659652072
CMNPD26113	-6.277154365	-1.591473637	4.685680729
CMNPD26114	-6.273642734	-1.621003719	4.652639015
CMNPD28880	-6.744555586	-1.640520551	5.104035035
CMNPD28881	-6.7406249	-1.552061463	5.188563437
CMNPD28882	-6.894214471	-1.574662979	5.319551492
CMNPD28883	-6.552573452	-1.49444704	5.058126412
CMNPD28884	-6.735437863	-1.67443956	5.060998303
CMNPD28885	-6.425510641	-1.311900458	5.113610183
CMNPD28886	-6.568858114	-1.684824246	4.884033868
CMNPD28902	-6.171887613	-2.771723442	3.400164171
CMNPD28903	-6.227971939	-1.599719507	4.628252432
CMNPD28904	-5.65043122	-2.146211748	3.504219472
CMNPD28906	-5.830123054	-1.966458416	3.863664638

CMNPD28931	-6.328313156	-1.562960444	4.765352712
CMNPD28932	-6.27141113	-1.546983272	4.724427858
CMNPD28933	-6.446094431	-1.647302176	4.798792256
CMNPD28934	-6.427755309	-1.654447889	4.77330742
CMNPD28965	-6.490949157	-2.411931059	4.079018098
CMNPD28966	-6.543180621	-2.425182738	4.117997883
CMNPD29067	-5.417925054	-1.240969593	4.176955461
CMNPD29067	-5.417925054	-1.240969593	4.176955461
CMNPD29068	-5.461853504	-1.309887359	4.151966145
CMNPD29070	-5.412431889	-1.83038455	3.582047339
CMNPD30304	-5.999289246	-1.521445101	4.477844145
CMNPD30305	-6.24751707	-2.002141812	4.245375258
CMNPD30637	-6.466045285	-2.477035419	3.989009865
CMNPD30638	-6.482700022	-2.321265671	4.161434351
CMNPD30639	-6.360022327	-2.301668021	4.058354306
CMNPD30643	-5.642822096	-0.590911584	5.051910512
CMNPD21959	-5.581493862	-2.370420886	3.211072976
CMNPD14698	-6.244811713	-2.710461331	3.534350382

.

TABLE 5.15 MARINE SPONGES DFT TABLE

COMPOUND IDENTIFIER	HOMO ENERGY (eV)	LUMO ENERGY (eV)	Binding gp energy (eV)
CMNPD5568	-5.902686603	0.4391334754	6.341820078
CMNPD966	-6.26598844	-1.339592683	4.926395757
CMNPD2771	-6.710569909	-1.641600299	5.06896961
CMNPD2773	-6.677358125	-1.260146282	5.417211843
CMNPD6139	-7.107777694	-3.685228066	3.422549628
CMNPD6245	-6.344337133	-0.3552842705	5.989052862
CMNPD6261	-6.677171999	1.286427051	7.96359905
CMNPD6756	-5.934514144	-2.973990669	2.960523475

CMNPD6757	-6.262255852	-2.969566095	3.292689757
CMNPD14212	-6.465627046	-3.054179396	3.41144765
CMNPD14213	-6.044394317	-2.165372654	3.879021663
CMNPD10387	-5.49524053	-1.050389662	4.444850868
CMNPD11152	-6.544164858	-1.134547444	5.409617414
CMNPD20297	-6.232081948	1.139729855	7.371811803
CMNPD5012	-6.553890484	-0.7685127661	5.785377718
CMNPD6877	-5.883818763	-1.880204812	4.003613951
CMNPD11844	-6.33460552	-1.467872115	4.866733405
CMNPD11119	-6.179353604	-1.344283111	4.835070493
CMNPD20296	-6.484437742	-0.4284992606	6.055938481
CMNPD7623	-6.314280238	-2.051649415	4.262630823
CMNPD3038	-6.183380891	-1.608134088	4.575246803
CMNPD8365	-5.877799874	0.458459283	6.336259157
CMNPD1065	-6.194366949	-1.734640698	4.459726251
CMNPD5567	-5.73662768	0.5064120267	6.243039707
CMNPD5569	-5.950851595	0.5055684733	6.456420069
CMNPD8981	-7.524933339	-1.740632648	5.78430069
CMNPD8982	-6.998336168	-1.719020267	5.279315902
CMNPD878	-7.103097061	-2.411924528	4.691172533
CMNPD967	-6.274699353	-1.344593321	4.930106032
CMNPD2769	-5.923252434	0.5750753661	6.4983278
CMNPD2772	-7.019430173	-1.74356903	5.275861142
CMNPD6872	-5.556424816	-0.7465327585	4.809892057
CMNPD7692	-6.769635788	0.4028846265	7.172520415
CMNPD9619	-5.892391442	-0.619316475	5.273074967
CMNPD10435	-5.895300885	-0.6983816438	5.196919241
CMNPD11223	-6.0272144	-1.457695324	4.569519076
CMNPD25205	-6.213974395	-3.012512213	3.201462182
CMNPD25206	-5.82890752	-2.262887424	3.566020097
CMNPD25208	-6.102094728	-1.296701803	4.805392925
CMNPD25209	-6.015130906	-1.384666732	4.630464174
CMNPD9738	-5.99919836	-1.739532764	4.259665597
CMNPD20295	-6.659668267	-0.4371356144	6.222532652
CMNPD5567	-5.73662768	0.5064120267	6.243039707
CMNPD5010	-6.635640873	-1.000840425	5.634800448

CMNPD5011	-6.667926382	-1.003157204	5.664769178
CMNPD6874	-5.551498192	-0.1530390849	5.398459107
CMNPD6875	-5.916474347	0.5160739781	6.432548325
CMNPD6876	-6.339811333	-0.8044998413	5.535311491
CMNPD6716	-5.669701516	1.837057329	7.506758845
CMNPD6896	-5.607156116	0.9322881085	6.539444224
CMNPD8324	-5.831512196	0.427733804	6.259245999
CMNPD11249	-5.672150542	-0.3178898217	5.35426072
CMNPD11843	-6.33522594	-1.727681111	4.607544829
CMNPD11117	-6.412799652	-1.595290308	4.817509344
CMNPD11118	-6.36531957	-2.146232428	4.219087142
CMNPD18101	-6.292184037	-1.477820875	4.814363162
CMNPD11153	-6.519782628	-0.997129879	5.522652749
CMNPD15143	-5.831702675	-0.7814332826	5.050269393
CMNPD10459	-5.963875787	-0.2852807696	5.678595018
CMNPD14268	-5.802980227	-0.9035972257	4.899383002

DENSITY FUNCTIONAL THEORY ANALYSIS

Density-functional theory (DFT) is a successful theory to calculate the electronic structure of atoms, molecules, and solids. Its goal is the quantitative understanding of material properties from the fundamental laws of quantum mechanics. Density functional theory (DFT) finds increasing use in applications related to biological systems

TABLE 5.16 INTERACTION TABLE FOR MARINE BACTERIA

Compound Identifier	Hydrogen Bond (HB) interaction	Pi-sigma and mide interaction	alkyl interaction	Carbon- Hydrogen Interaction
CMNPD30087	LEU113,ASN114,GLU110,ARG115,		ARG115,ARG140,GLU689,ARG141:NH1,LYS204	ARG115
CMNPD30086	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,LEU113,GLY118,ARG115	LYS204	ARG115,GLU116,GLU689,ARG141,ASP300,ARG162,LYS204	

CMNPD28614	LEU113,GLU110,ASN114,ARG115,ILE112,PHE119,ALA120,GLY122,MET123		ARG115,GLU116,ARG140,GLU689,ARG154,GLU791,LYS271	
CMNPD28613	LEU113,GLU110,ARG115,GLU116,GLY118,LYS132,MET130,GLU135		ARG115,GLU116,ARG140,GLU689,ARG141,ASP300,LYS204,GLU417	GLU116,
CMNPD28608	LEU113,GLU110,ASN114,GLU110,ARG115,ILE112,GLU116,LEU113,GLY118,PHE119,ALA120		ARG115,GLU116,ARG140,GLU689,ASP138,LYS204,ASP787,GLU417,	
CMNPD28607	LEU113,GLU110,ASN114,ARG115,GLU116,LEU113,GLY118,PHE119,ALA120,PRO124	MET 922	ARG115,GLU116,ARG140,GLU791,ARG226,LYS253,GLU417,LYS640,GLU707,LYS924	
CMNPD28606	LEU113,GLU110,ASN114,ARG115,GLU116,ILE112,GLU116,GLY118,ARG115,PHE119,GLU127,MET130,PHE128		ARG115,GLU116,ASP129,ARG140,ASP138,ARG154,ASP155,LYS253,GLU417,LYS656	ARG154
CMNPD28605	LEU113,GLU110,ASN114,ARG115,GLU116,ILE117,GLY118,PHE119,ARG115,PHE128,CYS126,GLU135,ASP133	LYS627	ARG115,ARG140.ARG141,GLU116,ASP129,GLU689,ASP138,ARG154,GLU223,ARG537,LYS627	
CMNPD28508	LEU113,GLU110,ARG115,ILE112,GLU116,GLY118,ARG115,PHE119,GLU116,MET130,VAL131,MET130,GLU135,VAL136,ASP138	ARG115,ARG140,GLU116	ARG115,ARG140,GLU116,ASP129,GLU689,ARG154,ASP300,LYS204,GLU223,LYS253,LYS271,LYS627,GLU674	

CMNPD28507	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,LEU113,GLY118,PHE119,ARG115,ALA120,GLY122,MET123,PRO124,ASP129,MET130		ARG115,GLU116,ARG140,ASP129,ARG141,ASP138,ARG154,ASP300,ARG162,LYS204,GLU223,LYS253	
CMNPD28506	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,ILE117,GLY118,PHE119,ALA120,GLY122,MET123,PRO124,PHE128,MET130,VAL131,PHE139,LEU144	MET922,PHE930	ARG115,GLU116,ARG140,ASP129,GLU689,ARG141,ASP138,ARG154,ASP155,LYS204,GLU223,LYS253,ARG335	GLU223,LYS253
CMNPD25829	LEU113,GLU110,ASN114,ARG115,LYS111,GLU116,LEU113,ILE117,GLY118,ARG115		ARG115,GLU116,ARG140,ASP129,ARG141,ASP300,LYS204,GLU223,LYS253,LYS776	
CMNPD30117	LEU113,ASN114,GLU110,ARG115,ILE112,GLU116,ILE117,GLY118,PHE119,ALA120,MET123,PRO124,MET130	ARG140	ARG115,GLU116,ARG140,GLU689,ARG141,ASP300,ARG162,LYS204,GLU791	
CMNPD27173	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,LEU113,GLY118,PHE119,GLY122,MET123	GLU116	ARG115,GLU116,ARG140,ASP129,GLU689,LYS204,GLU223,LYS253,ASP478	
CMNPD21772	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,ILE117,ASN114,GLY118,ALA120,MET123,PHE128,VAL131		ARG115,GLU116,ARG140,ASP129,ARG154,ASP300,LYS204,GLU223,LYS253,ARG979	ARG979
CMNPD27241	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,ILE117,GLY118,P		ARG115,GLU116,ARG140,GLU689,ASP129,A	GLU116

	HE119,GLU116,MET123		RG154,ASP155,LYS204,GLU223,LYS253	
CMNPD25827	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,ILE117,PHE119,GLU116,ILE121,GLU127,CYS126	,LYS253	GLU116,ASP129,GLU689,ASP138,ARG140,LYS204,LYS253,LYS271,ASP478,GLU417	
CMNPD30237	LEU113,ASN114,ARG115,ILE112,GLU116,GLY118,PHE119,ALA120,GLY122,MET130,GLU135:N,LYS290		ARG115,GLU116,ARG140,ASP129,ARG154,ARG162,LYS204,GLU223,LYS253,LYS253,GLU707	
CMNPD21962	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,LEU113,GLY118,PHE119,ALA120,ILE121,VAL125	MET 722,MET 922	ARG115,GLU116,ARG141,GLU689,ASP138,ARG154,ARG162,LYS204,GLU223,LYS271	VAL 850
CMNPD21961	LEU113,ASN114,GLU110,ASN114,ARG115,ILE112,GLU116,PHE119,ALA120,ILE121,GLY118,PHE128,ARG140	MET 922	GLU116,ARG140,ARG115,ARG141,ARG162,ASP155,LYS204,GLU223,ARG537,GLU547,ARG612	
CMNPD21959	LEU113,GLU110,ASN114,ARG115,LYS111,ARG115,ASN114,GLU116,ALA120,ILE117,ILE121,MET123,GLU127,PRO124,ASP129		GLU116,ASP129,ARG115,ARG140,ASP138,ASP300,ASP155,ARG162,LYS204,LYS253,LYS271,ASP478,GLU417	
CMNPD14698	LEU113,GLU110,ASN114,ARG115,ILE112,GLU116,LEU113,ILE117,GLY118,PHE119,ARG115,ALA120,ILE117,GLY122,MET123,GLY118,PH	MET 922	GLU116,ASP129,ARG115,ARG140,ARG154,ASP155,GLU791,GLU223,ASP787,LYS253,LYS271,ASP478,GLU417,LYS627LYS640,GLU689	

	E128,CYS147,LEU153, ARG154			

TABLE 5.17 INTERACTION TABLE FOR MARINE FUNGI

Compound Identifier	Hydrogen Bond (HB) interaction	Pi-sigma and mide interaction	alkyl interaction	Carbon- Hydrogen Interaction
CMNPD22236		:ILE932	:ILE800,:ILE848,:ILE932,	
CMNPD15724	:LYS802,:SER854		:LYS802	:SP810
CMNPD15725	:LYS802,	:ILE848,:MET922	:LYS802	:SP810
CMNPD14250			:RG852,:MET772,:TRP780,:HIS855,	:SER774,:VAL850
CMNPD14251	:SER854,:RG770		:PRO778,:ILE848,:ILE932	
CMNPD30821		:VAL850,:MET922	:VAL851	
CMNPD18724	:SER774		:TRP780,:ILE800,:VAL850,:MET922,:ILE932	:VAL850
CMNPD18725	:SER854		:ILE800,:ILE932	:SER919
CMNPD28911	:LYS802,:VAL851,:SER854:	:ILE848	:VAL850,:MET922,:MET772,:PRO778,:TRP780,:ILE932	:VAL850,:HIS855
CMNPD25904	:GLN859	:ILE932	:VAL850,:TRP780,:ILE800	:VAL850,:TYR836

CMNPD26113	:RG770	:MET772,:ILE848,:ILE932	:ILE800,:ILE848,:ILE932	
CMNPD26114	:GLN859		:VAL851	
CMNPD28880	:SER774,:RG770		:VAL850,:MET922,:TRP780	:GLU849
CMNPD28881	:MET922	:TYR836	:VAL850,:MET922,:ILE800,:ILE848,:TRP780	
CMNPD28882	:VAL851,:SER854	:TRP780,:MET922	:ILE800,:VAL850,	:VAL851,:SER854
CMNPD28883	:SER854,:VAL851,			
CMNPD28884		:ILE932	:ILE932,:TYR836,:ILE800,:ILE848	:SER854
CMNPD28885	:VAL851		:VAL850,:ILE800,:VAL850,:TRP780	:SER854,:GLN859
CMNPD28886	:SER774		:VAL850,:MET922,:ILE800,:ILE932	:GLU849
CMNPD28902	:LYS802,:SER854	:MET772,:MET922,:ILE932	:ILE800,:ILE848,:ILE932,:VAL850	:SER774,:VAL851,:SER854
CMNPD28903	:VAL851,:SER854,:GLN859,			:SP810
CMNPD28904	:VAL851,:SER854,:GLN859		:VAL851	
CMNPD28906			:PRO778,:VAL850,:ILE932	:SER854,:SER774,:SER774
CMNPD28931	:VAL851,:SER854			

CMNPD28932	:RG770	:ILE932	:VAL850,:MET922,:TRP780,:ILE800,:ILE848	
CMNPD28933	:VAL851,:SER854	:ILE932	:VAL851,:VAL850,:MET922,:ILE800	
CMNPD28934	:VAL851,:SER854			
CMNPD28965	:VAL851,:SER854,:VAL851			
CMNPD28966	:VAL851,:SER854			:SP810
CMNPD29067	:LYS802		:LYS802	:SP810
CMNPD29068	:VAL851,:SER854		:VAL851,:LYS802	:SER774
CMNPD29070	:SER774,:VAL851,:SER854			
CMNPD30304	:SER854,:VAL851			:SER919
CMNPD30305	:VAL851,:GLN859		:SER919	:SER919
CMNPD30637	:SER854,:VAL851		:VAL851	:SER919
CMNPD30638	:GLN859			:VAL851,:SER854
CMNPD30639	:VAL851			:SER919
CMNPD30643	:VAL851,:SER854		:VAL851	
CMNPD21959	:GLN859,:VAL851			:SER774
CMNPD14698	:VAL851,:SER854,:GLN859			

TABLE 5.18 INTERACTION TABLE FOR SPONGES

Compound Identifier	Hydrogen Bond (HB) interaction	Pi-sigma and mide interaction	alkyl interaction	Carbon- Hydrogen Interaction
CMNPD5567		ILE848 , ILE932,	ILE848,ILE932,ILE848,ILE932,MET772,PRO778,ILE800,ILE848,MET922,VAL850,VAL851,ILE932,VAL851	GLU849
CMNPD5568	:LYS802,:GLN859		MET772,TRP780,PRO778,LYS802,VAL850,VAL851,ILE932,MET772,PRO778	LYS802,GLN859
CMNPD5569	:RG770	THR856,RG770	ILE932,ILE848,TYR836	TYR836
CMNPD8981		VAL850	VAL851, MET922,	
CMNPD8982	:MET922,:PHE930	ILE932	VAL851,VAL851,VAL851,MET922	GLU849
CMNPD878	:MET922,:PHE930	ILE932:CG2	VAL851,MET922	GLU849:
CMNPD966	:RG770,:MET772		PRO778,PRO778,MET772,LYS802,LYS802	
CMNPD967	:ILE800,:ILE848	ILE848,ILE932,	HIS855,ILE800	

CMNPD2769		MET922:CE	VAL850, MET922, TRP780, VAL850	
CMNPD2771	:RG770,CMNPD2771	MET922,	MET922,ILE932,PHE930	SER774
CMNPD2772	:RG770,:GLN859		MET922	
CMNPD2773	:RG770,:GLN859,		ILE800,VAL850,MET772,TRP780	VAL851,SER854
CMNPD5149		TYR836		
CMNPD6139	:VAL851,:SER854	ILE932,,TYR836	VAL850,MET922,TRP780,ILE848	
CMNPD6245	:RG770,:SER854,		MET922:SD,MET772,ILE800,ILE848,ILE932	
CMNPD6261	:RG770,:GLN859,:SER854		ILE800,VAL850,VAL851,MET772,MET922,ILE932,ILE848,ILE932,TRP780,TYR836	
CMNPD6756	:VAL851	ILE800,,MET922,TYR836	ILE800,ILE848,ILE932,VAL850,ILE932	VAL851,SER854,GLU849
CMNPD6757	:VAL851	MET922	VAL850,ILE800,ILE848,ILE932,TRP780,	VAL851,SER854,

CMNPD7692			MET922,ILE800,VAL850 ,ILE932,MET772	
CMNPD14212	:LYS802,:SER854,:SER 854	MET922,ILE932	LYS802,ILE848,ILE800, MET922	:SER919,SN920,:SP933 ,
CMNPD14213	:RG770,:VAL851,:SER8 54,	TYR836	HIS855,VAL850,MET92 2,VAL850,VAL851,ILE93 2	GLU798
CMNPD9619		MET922	MET922 ,ILE932,VAL851,ILE932, TYR836,PHE930,VAL85 0	SP810,TYR836
CMNPD10387	:RG770,:SER854,:GLU8 49,	ILE932	ILE800	VAL851,SER854,
CMNPD10435	:GLU849,	MET922	VAL851 ILE932 ILE800 ILE932 TYR836 PHE930 VAL850 ILE932	SER854,SP933
CMNPD11152	:SER774,:LYS802	ILE932	MET772 ,MET922, ILE800 ,MET922	SP933
CMNPD11223			VAL850,MET922,ILE932 ,MET772,ILE800,VAL85 1	HIS855
CMNPD25025	VAL851,SER854	ILE848,MET922	VAL850,MET772,ILE800 ,ILE932	

CMNPD25206	GLN859:NE2	MET772 ,MET922:,ILE932	RG852,ILE800,VAL850, VAL851,MET922,ILE932	
CMNPD25280			VAL850	
CMNPD25290	GLU849		VAL850	GLU849,VAL851
CMNPD9738			MET772,MET922,MET922	
CMNPD20295			VAL850,MET922,ILE800 ,ILE932,ILE848,ILE800, LYS802,ILE848	
CMNPD20297	RG770,GLN859,SER854		VAL850,VAL851,MET922,MET772,MET922,ILE932,ILE848,ILE932,PRO778,ILE800,LYS802,ILE848,TRP780,TYR836	
CMNPD5010	GLN859,		VAL850,MET922,ILE848 ,ILE932,TRP780,HIS855	
CMNPD5011	GLN859		ILE800,ILE848,VAL850,ILE932,MET922,ILE800,ILE848,ILE932	
CMNPD5012	GLN859:NE2		MET922,CMNPD5012,HIS855	

CMNPD6874	MET922,:PHE930	MET922	ILE800,MET922,ILE932,VAL850,TRP780,PHE930	
CMNPD6875			:VAL850,:MET922,:MET922,:ILE800,:TRP780,:ILE932	
CMNPD6876	SER854,VAL851	MET922	:VAL851,:ILE932,:TYR836,:PHE930,:VAL850	
CMNPD6716			:MET922,:ILE848,:ILE932,:VAL850,:VAL851,:TYR836,:MET922,	
CMNPD6877	RG770,		:VAL850,:MET922,:ILE932,:ILE800,:ILE932,:MET772,:TRP780	
CMNPD6896	MET922,PHE930	MET922	:VAL851,:ILE932,:MET772,:MET922,:VAL850,:TRP780,:PHE930	
CMNPD8324	MET772,ILE800,ILE848		:ILE932,:VAL851,:MET772,:PRO778,:ILE800,:ILE848,:TYR836 ,:MET922	PRO778
CMNPD11249	RG770,	:ILE932	:TRP780,:PRO778,:ILE800,:LYS802	

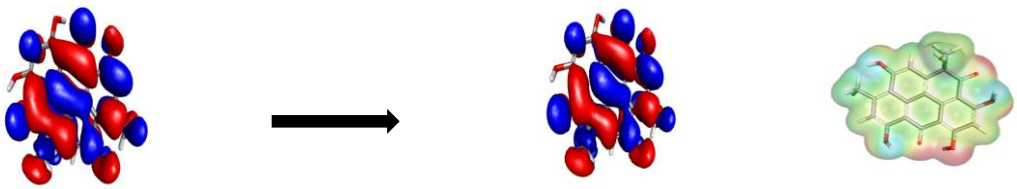
CMNPD11843	:SER774:OG		:ILE932	:HIS917,:SER919
CMNPD11844	:TYR836,:SER854		:ILE800,:ILE848,:ILE932,:TRP780	:SP810,:TYR836
CMNPD11117		ILE932		
CMNPD11118			:VAL850,:VAL851,:MET922	
CMNPD11119	:RG770,		:MET922,:ILE932,	
CMNPD18101			:VAL850,:MET922,:TRP780,:VAL850,	
CMNPD20296	:RG770,:GLN859,:ILE800,:ILE848	:TYR836	:VAL850,:MET772,:ILE800,:MET922,:ILE932,:VAL851,:TYR836	
CMNPD11153			:VAL851,:ILE932,:TYR836,:VAL850,	
CMNPD7623	:RG770,		:VAL850,:ILE932,	
CMNPD1065	:MET922	:MET922	:VAL850,:MET922,:ILE800,:VAL851,:TRP780,:PHE930	

CMNPD3038	:RG770		:ILE800,:MET922,:ILE932,:ILE848,:ILE932,:TYR836	:SER854
CMNPD15143	:RG770		:MET772,:ILE800,:ILE932,:VAL851,:ILE932,:TYR836,:VAL850,	:SN920,:SP933
CMNPD10459		:TRP780,:TYR836	:VAL850,:MET922,:VAL850,	:GLU849
CMNPD14268	:TYR836,:SP933	:ILE932	:VAL851,:ILE932,:MET772,:MET922,:TYR836,:PHE930,:ILE800	:VAL851,:SER854
CMNPD8365	:LYS802		:VAL850,:MET922,:ILE932,:ILE800,:ILE932,:MET772,:PRO778,:TRP780	

sThis table refers as interaction table where the amino acid are high, the amino acids are lysine, methionine, proline, valine Charged amino acid side chains can form ionic bonds, and polar amino acids are capable of forming hydrogen bonds. Hydrophobic side chains interact with each other via weak van der Waals interactions. The vast majority of bonds formed by these side chains are noncovalent.

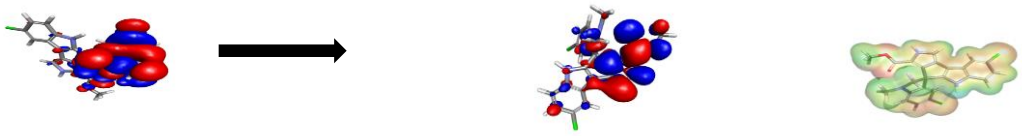
MOLECULAR ORBITAL OF MARINE BACTERIA

FIGURE 5.1.1 CMNPD14698



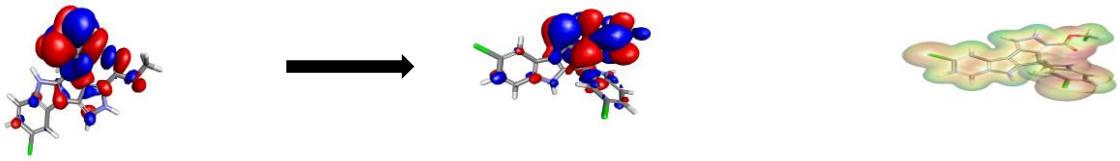
HOMO -6.244811713 **(eV) BINDING GAP ENERGY**3.534350382 **LUMO**-2.710461331 **(eV) EPS**

FIGURE 5.1.2 CMNPD14698



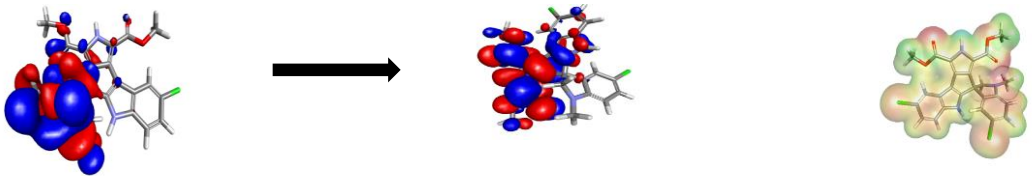
HOMO -5.581493862 **(eV) BINDING GAP ENERGY** 3.211072976 **LUMO**-2.370420886 **(eV) EPS**

FIGURE 5.1.3 CMNPD21959



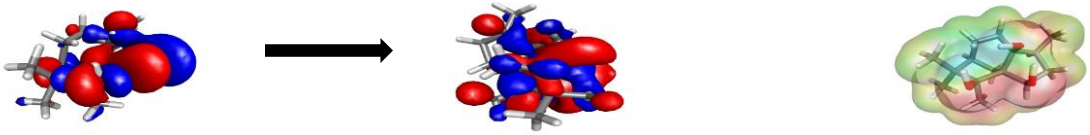
HOMO -5.018420355 **(eV) BINDING GAP ENERGY** 3.628608491**LUMO** -1.389811864 **(eV) EPS**

FIGURE 5.1.4 CMNPD21961



HOMO -5.106532498 **(eV) BINDING GAP ENERGY** 3.666474786**LUMO** -1.440057712 **(eV) EPS**

FIGURE 5.1.5CMNPD21962

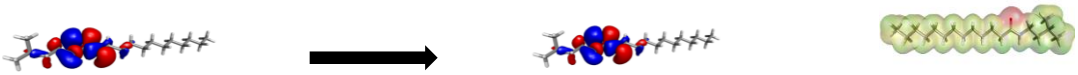


HOMO -5.094585877 **(eV) BINDING GAP ENERGY** 2.901505488 **LUMO** -2.193080389 **(eV) EPS**

FIGURE 5.1.6 CMNPD23280

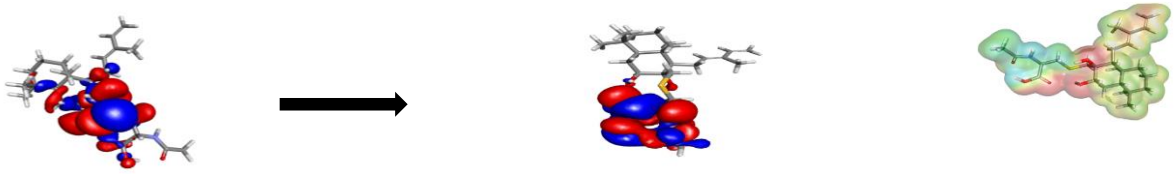
HOMO -6.24598779 **(eV)** **BINDING GAP ENERGY** 6.570373789 **LUMO** 0.324385999 **(eV)** **EPS**

FIGURE 5.1.7 CMNPD24388



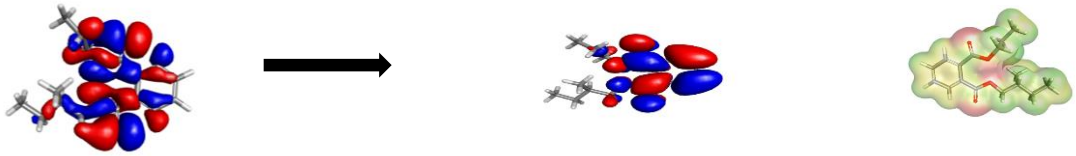
HOMO -5.842152941 **(eV)** **BINDING GAP ENERGY** 4.1923065**LUMO** -1.649846441 **(eV)** **EPS**

FIGURE 5.1.7 CMNPD25827



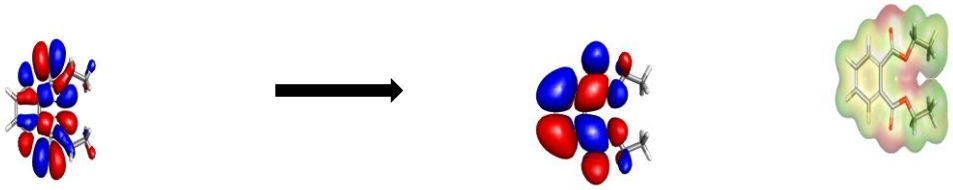
HOMO -6.840687745 **(eV)** **BINDING GAP ENERGY** 7.633048853 **LUMO** 0.7923611083 **(eV)** **EPS**

FIGURE 5.1.8 CMNPD25829



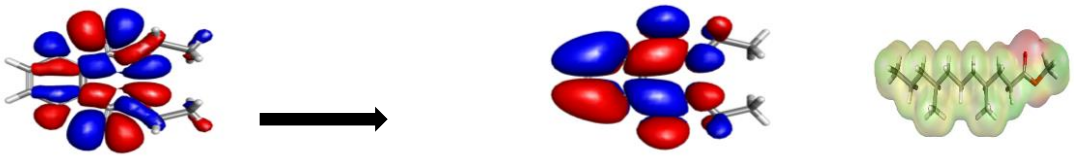
HOMO -5.868635891 **(eV)** **BINDING GAP ENERGY** 4.473108273 **LUMO** -1.395527618 **(eV)** **EPS**

FIGURE 5.1.9 CMNPD27172



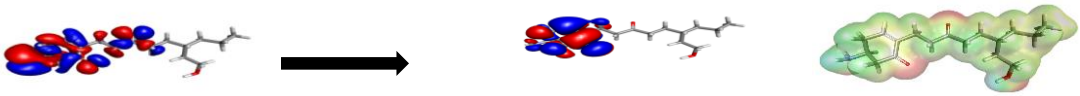
HOMO -7.408882436 **(eV)** **BINDING GAP ENERGY -** 5.405887275 **LUMO** -2.002995161 **(eV)** **EPS**

FIGURE 5.1.10 CMNPD27173



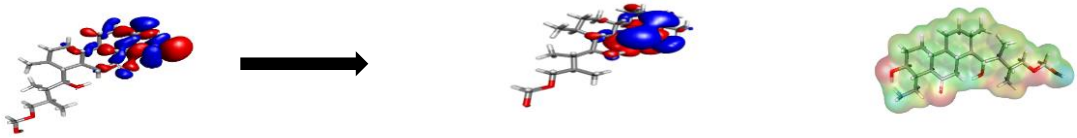
HOMO -7.450574653 **(eV)** **BINDING GAP ENERGY** 5.417711988 **LUMO** -2.032862665 **(eV)** **EPS**

FIGURE 5.1.11 CMNPD27241



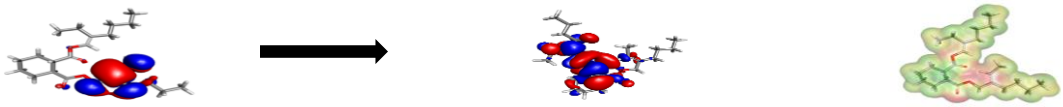
HOMO -7.366528166 **(eV)** **BINDING GAP ENERGY** 6.992833479 **LUMO** -0.3736946867 **(eV)** **EPS**

FIGURE 5.1.12 CMNPD28506



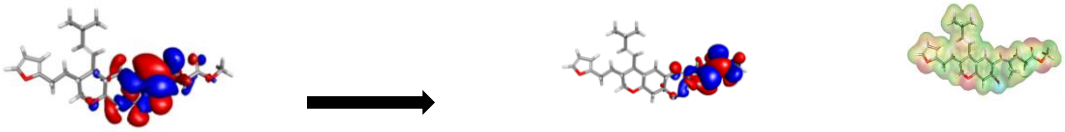
HOMO -6.251152241 **(eV)** **BINDING GAP ENERGY** 4.758681293 **LUMO** -1.492470948 **(eV)** **EPS**

FIGURE 5.1.13 CMNPD28507



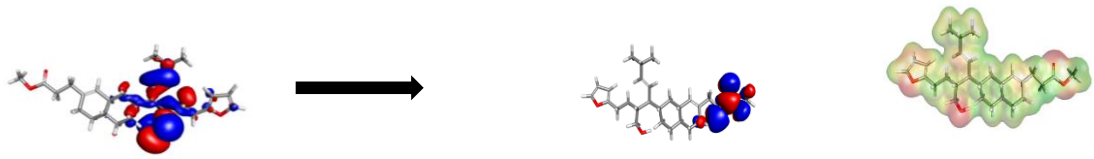
HOMO -6.050139188 **(eV)** **BINDING GAP ENERGY** 4.930189026 **LUMO** -1.119950161 **(eV)** **EPS**

FIGURE 5.1.14 CMNPD28508



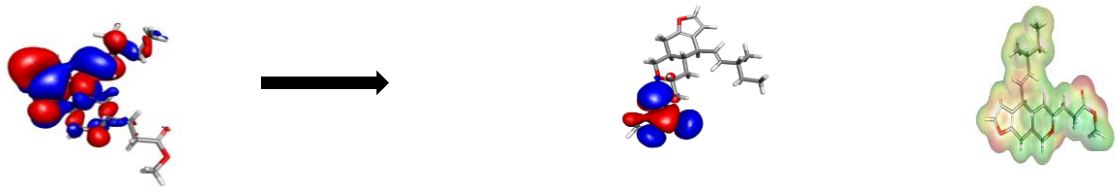
HOMO -5.898415502 **(eV)** **BINDING GAP ENERGY** 5.295033206 **LUMO** -0.6033822961 **(eV)** **EPS**

FIGURE 5.1.15 CMNPD28605

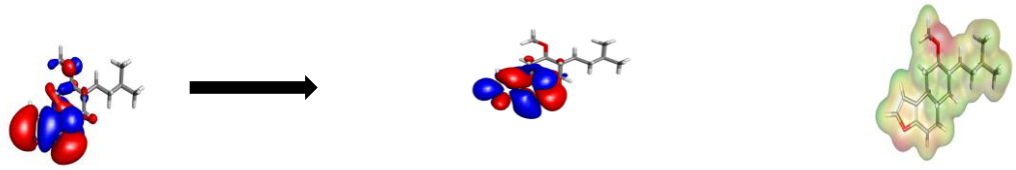


HOMO -5.988381557 **(eV)** **BINDING GAP ENERGY** 5.530412079 **LUMO** -0.4579694779 **(eV)** **EPS**

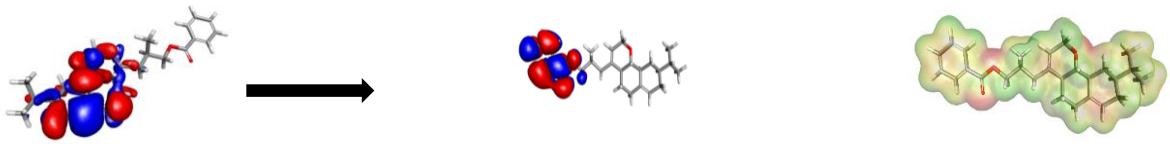
FIGURE 5.1.16 CMNPD28606



HOMO -6.032195719 **(eV)** **BINDING GAP ENERGY** 5.620617867**LUMO** -0.4115778522 **(eV)** **EPS** **FIGURE 5.1.17 CMNPD28607**

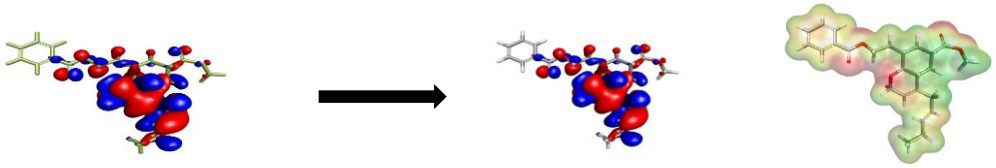


HOMO -5.943751325 **(eV)** **BINDING GAP ENERGY** 5.409671836 **LUMO** -0.5340794887 **(eV)** **EPS** **FIGURE 5.1.18 CMNPD28608**



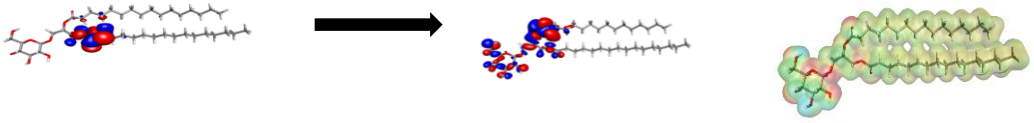
HOMO -5.563089432 **(eV)** **BINDING GAP ENERGY** 5.119078313 **LUMO** -0.4440111186 **(eV)** **EPS**

FIGURE 5.1.19 CMNPD28613



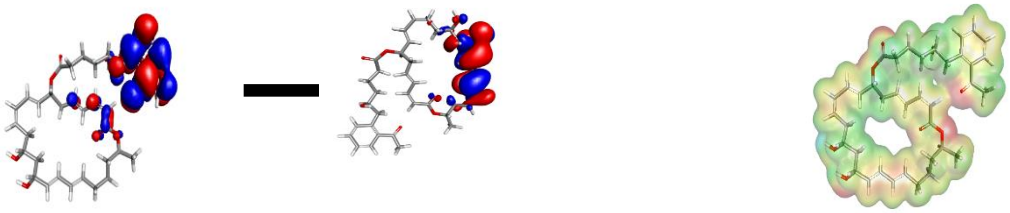
HOMO -6.056798361 **(eV)** **BINDING GAP ENERGY** 4.497910103 **LUMO** -1.558888259 **(eV)** **EPS**

FIGURE 5.1.20 CMNPD28614



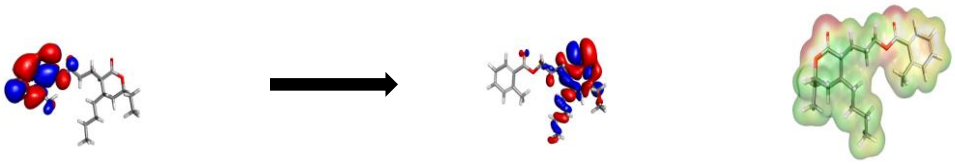
HOMO -6.209706831 **(eV)** **BINDING GAP ENERGY** 4.682953602 **LUMO** -1.526753229 **(eV)** **EPS**

FIGURE 5.1.21 CMNPD28694



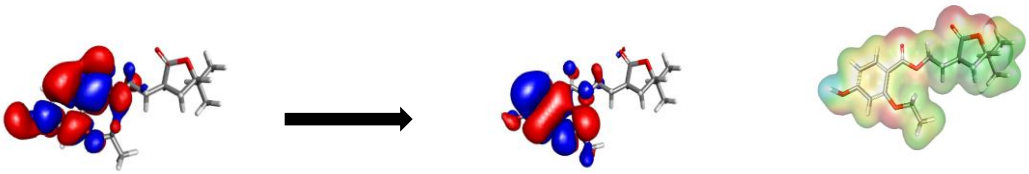
HOMO -7.119790982 **(eV)** **BINDING GAP ENERGY** 6.495210462 **LUMO** -0.6245805201 **(eV)** **EPS**

FIGURE 5.1.22 CMNPD29996



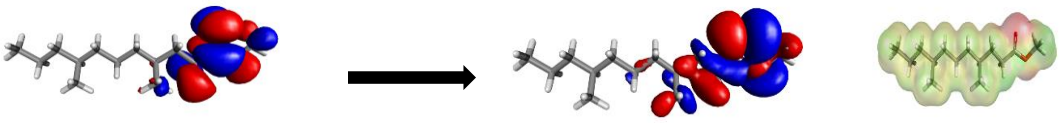
HOMO -5.746423511 **(eV)** **BINDING GAP ENERGY** 4.07832067 **LUMO** -1.668102841 **(eV)** **EPS**

FIGURE 5.1.23 CMNPD30086



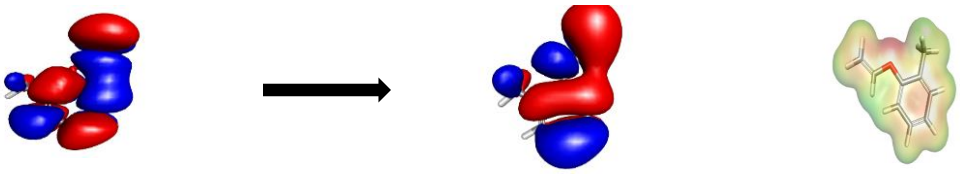
HOMO -6.720059341 **(eV)** **BINDING GAP ENERGY** 5.25228818**LUMO -** -1.467771161 **(eV)** **EPS**

FIGURE 5.1.24 CMNPD30087



HOMO -6.415817668 **(eV)** **BINDING GAP ENERGY** 4.817441044**LUMO** -1.598376624 **(eV)** **EPS**

FIGURE 5.1.25 CMNPD30117



HOMO -7.366528166 **(eV)** **BINDING GAP ENERGY** 6.992833479**LUMO** -0.3736946867 **(eV)** **EPS**

FIGURE 5.1.26 CMNPD30237

Figure 5.1 dft analysis of marine bacteria .

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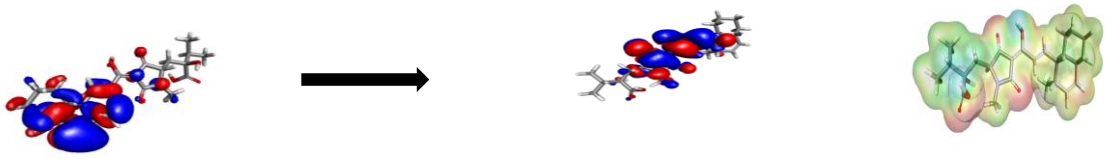
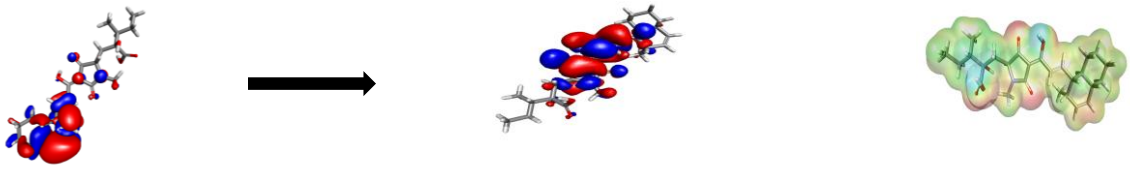


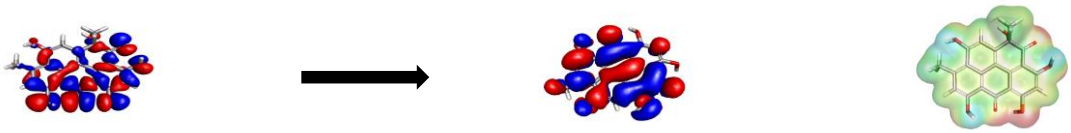
HOMO -6.272638362 (eV) BINDING GAP ENERGY 3.778400168 LUMO -2.494238194 (eV) EPS

FIGURE 5.2.1 CMNPD12450



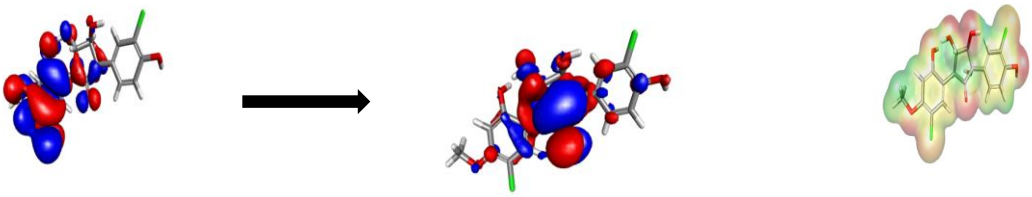
HOMO -6.270140083eV) BINDING GAP ENERGY 3.780402111LUMO -2.489737973 (eV) EPS

FIGURE 5.2.2 CMNPD12451



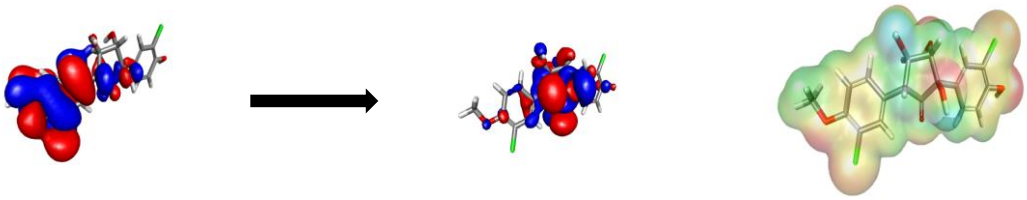
HOMO -6.270140083 (eV) BINDING GAP ENERGY 3.780402111 LUMO -2.489737973 (eV) EPS

FIGURE 5.2.3 CMNPD14698



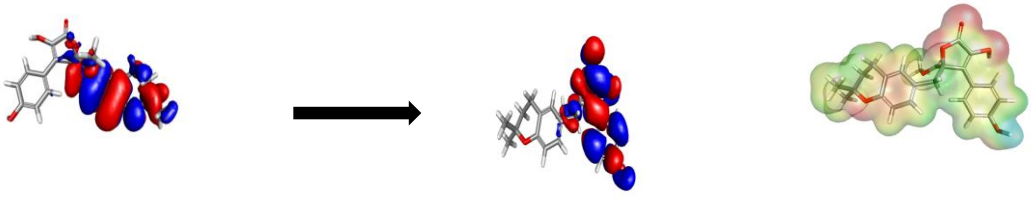
HOMO -6.244811713 (eV) BINDING GAP ENERGY 3.534350382LUMO -2.710461331 (eV) EPS

FIGURE 5.2.4 CMNPD15724



HOMO -6.546055778 (eV) BINDING GAP ENERGY 4.637504036LUMO -1.908551742 (eV) EPS

FIGURE 5.2.5 CMNPD15725

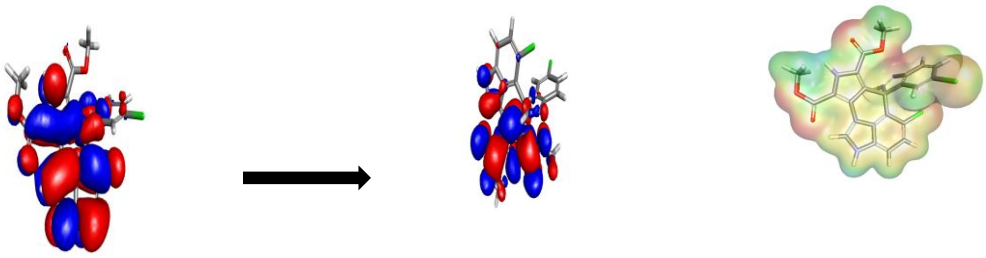


HOMO -6.357612486 (eV) BINDING GAP ENERGY 4.388880013 LUMO -1.968732473 (eV) EPS

FIGURE 5.2.6 CMNPD18724

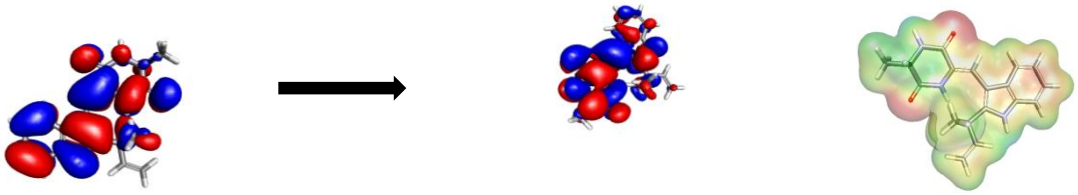
HOMO -5.743609853 (eV) BINDING GAP ENERGY 3.524591014 LUMO -2.219018839 (eV) EPS

FIGURE 5.2.7 CMNPD18725



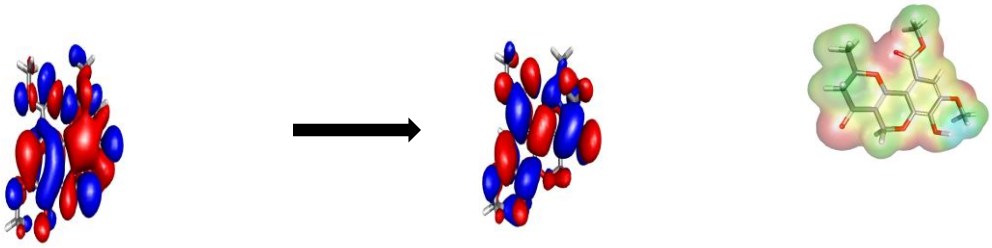
HOMO 4.388880013 (eV) BINDING GAP ENERGY -6.357612486 LUMO -1.968732473 (eV) EPS

FIGURE 5.2.8 CMNPD21959



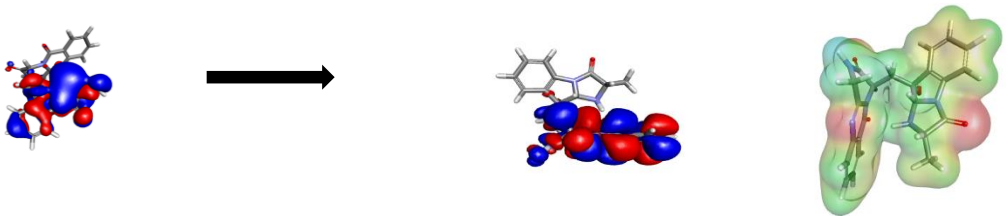
HOMO -5.581493862 (eV) BINDING GAP ENERGY - 3.211072976 LUMO -2.370420886 (eV) EPS

Figure 5.2.9 CMNPD22236



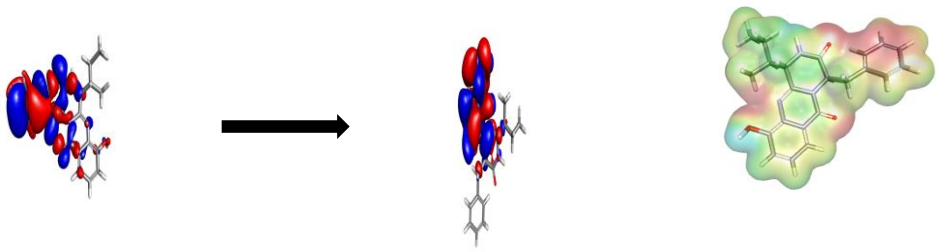
HOMO -5.478998045 (eV) BINDING GAP ENERGY 4.166847243 LUMO -1.312150803 (eV) EPS

FIGURE 5.2.10 CMNPD25904



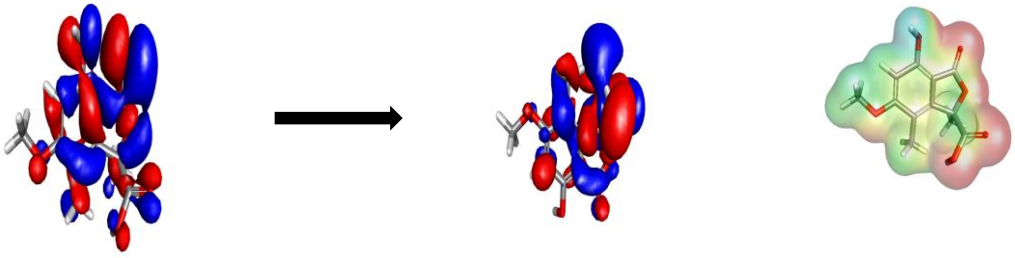
HOMO -6.086669946 (eV) BINDING GAP ENERGY 3.659652072 LUMO -2.427017875 (eV) EPS

FIGURE 5.2.11 CMNPD26113



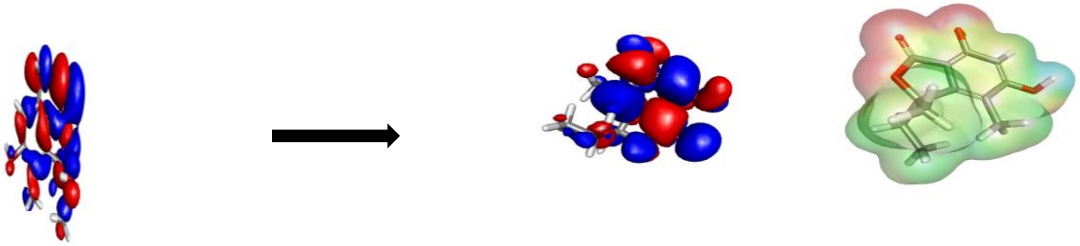
HOMO -6.277154365 (eV) BINDING GAP ENERGY - 4.685680729LUMO -1.591473637eV) EPS

FIGURE 5.2.12 CMNPD26114



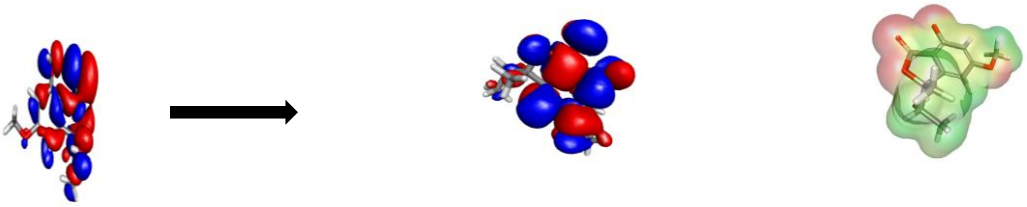
HOMO -6.273642734 (eV) BINDING GAP ENERGY 4.652639015LUMO -1.621003719 (eV) EPS

FIGURE 5.2.13 CMNPD28880



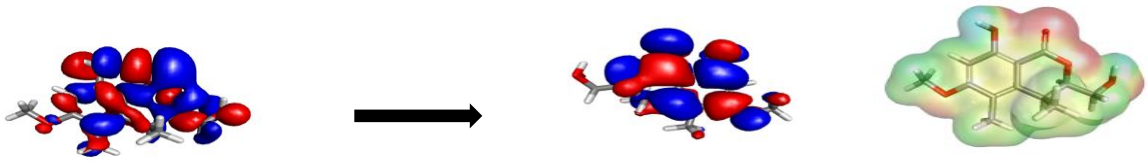
HOMO -6.744555586 (eV) BINDING GAP ENERGY 5.104035035LUMO -1.640520551 (eV) EPS

FIGURE 5.2.14 CMNPD28881



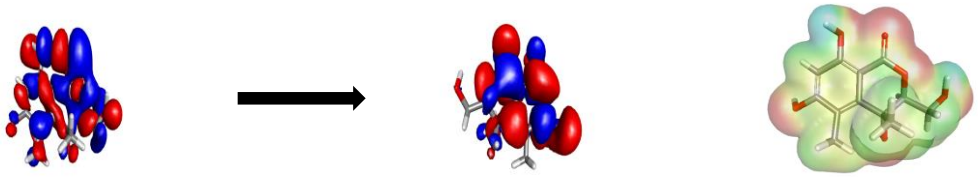
HOMO -6.7406249 (eV) BINDING GAP ENERGY 5.188563437 LUMO -1.552061463 (eV) EPS

FIGURE 5.2.15 CMNPD28882



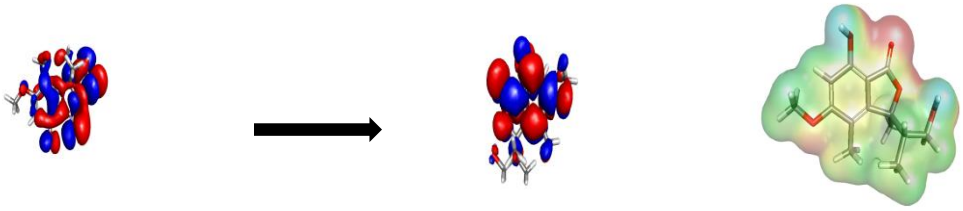
HOMO -6.894214471 (eV) BINDING GAP ENERGY 5.319551492LUMO -1.574662979 (eV) EPS

FIGURE 5.2.16 CMNPD28883



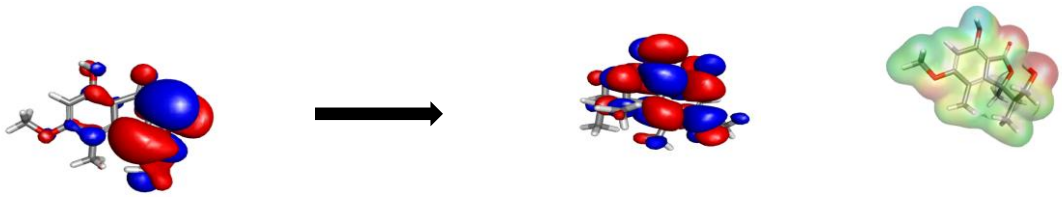
HOMO -6.552573452 (eV) BINDING GAP 5.058126412LUMO -1.49444704 (eV) EPS

FIGURE 5.2.17 CMNPD28884



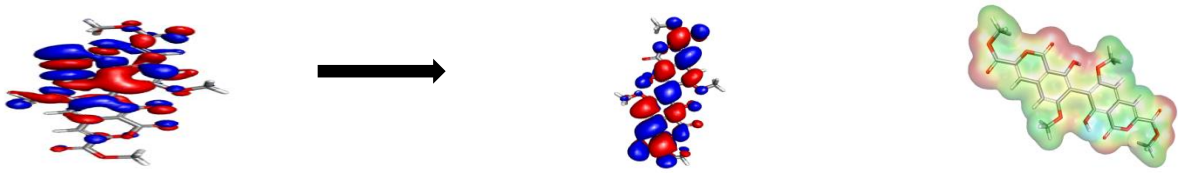
HOMO -6.735437863 (eV) BINDING GAP ENERGY 5.060998303LUMO -1.67443956 (eV) EPS

FIGURE 5.2.18 CMNPD28885



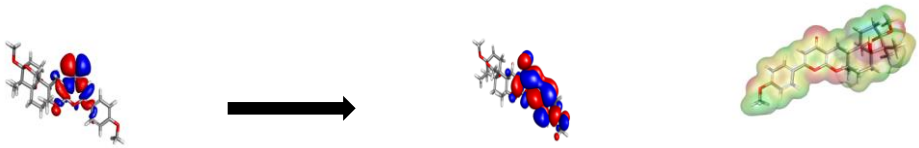
HOMO -6.425510641 (eV) BINDING GAP ENERGY 5.113610183LUMO -1.311900458 (eV) EPS

FIGURE 5.2.19 CMNPD28886



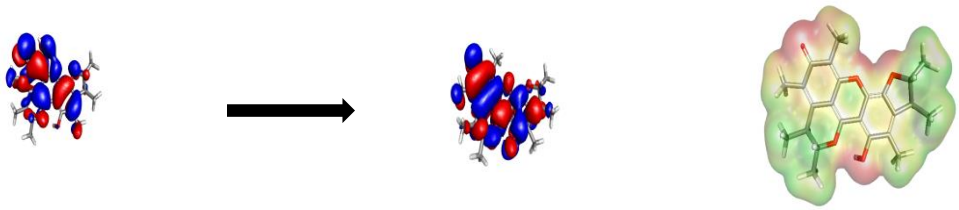
HOMO -6.568858114 (eV) BINDING GAP ENERGY 4.884033868LUMO -1.684824246 (eV) EPS

FIGURE 5.2.20 CMNPD28902



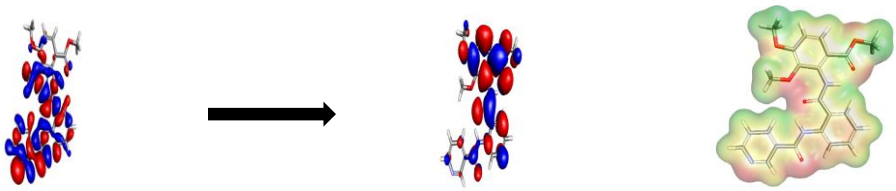
HOMO -6.171887613 (eV) BINDING GAP ENERGY 3.400164171LUMO -2.771723442 (eV) EPS

FIGURE 5.2.21 CMNPD28903



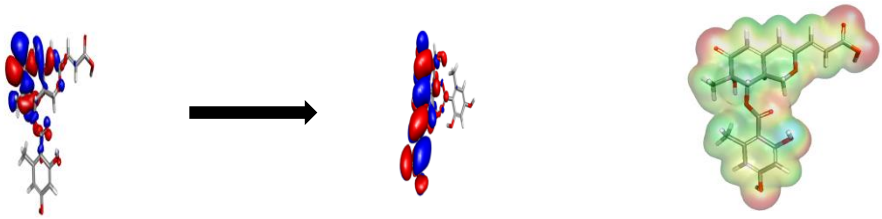
HOMO -6.227971939 (eV) BINDING GAP ENERGY 4.628252432LUMO -1.599719507 (eV) EPS

FIGURE 5.2.22 CMNPD28904



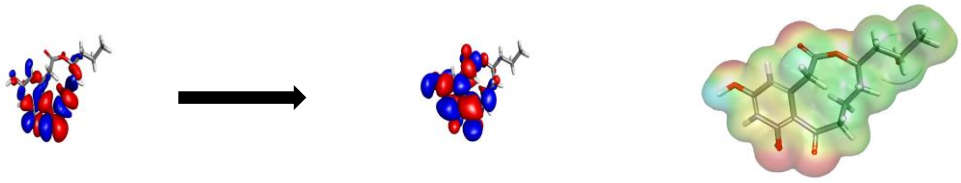
HOMO -5.65043122 (eV) BINDING GAP ENERGY - 3.504219472LUMO - -2.146211748 (eV) EPS

FIGURE 5.2.23 CMNPD28906



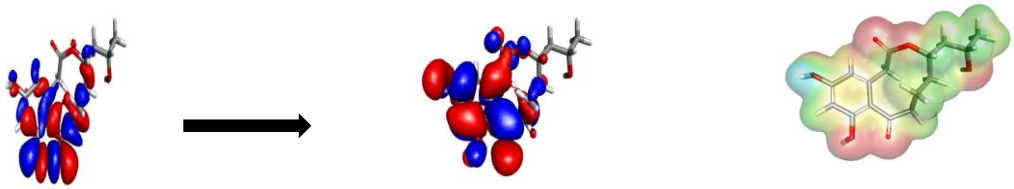
HOMO -5.830123054 (eV) BINDING GAP ENERGY 3.863664638LUMO -1.966458416 (eV) EPS

FIGURE 5.2.24 CMNPD28911



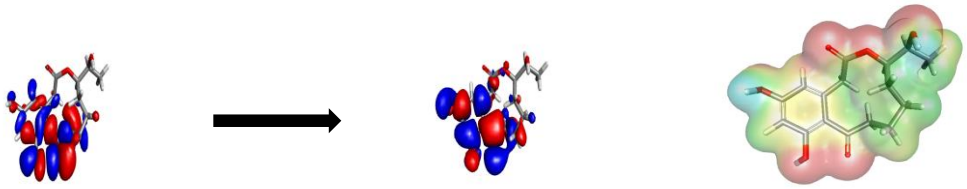
HOMO -6.416578499 (eV) BINDING GAP ENERGY 3.524483529LUMO -2.89209497 (eV) EPS

FIGURE 5.2.25 CMNPD28931



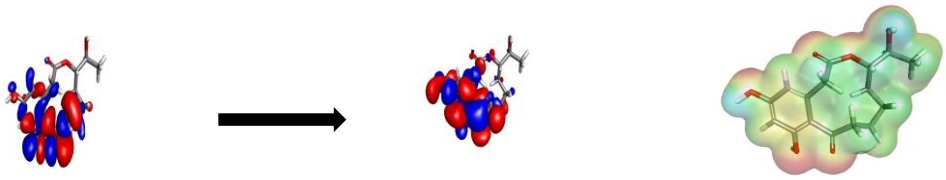
HOMO -6.328313156 (eV) BINDING GAP ENERGY 4.765352712 LUMO -1.562960444 (eV) EPS

FIGURE 5.2.26 CMNPD28932



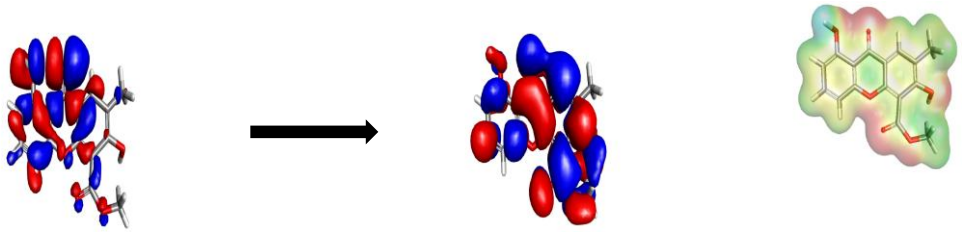
HOMO -6.27141113 (eV) BINDING GAP ENERGY 4.724427858 LUMO -1.546983272 (eV) EPS

FIGURE 5.2.27 CMNPD28933



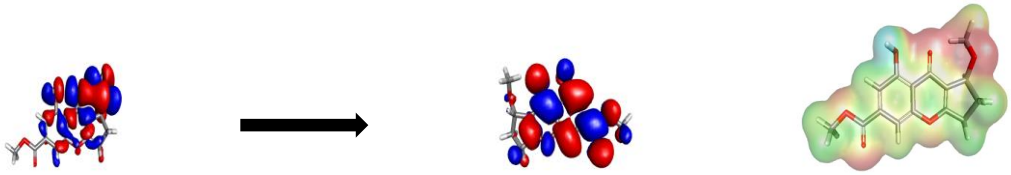
HOMO -6.446094431 (eV) BINDING GAP ENERGY 4.798792256 LUMO -1.647302176 (eV) EPS

FIGURE 5.2.28 CMNPD28934



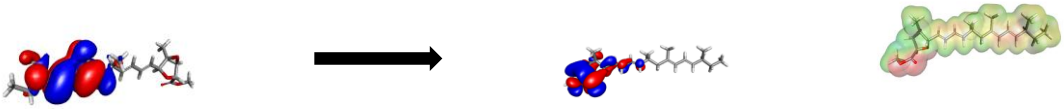
HOMO -5.12167 (eV) BINDING GAP ENERGY - 4.77330742 LUMO -1.654447889 (eV) EPS

FIGURE 5.2.29 CMNPD28965



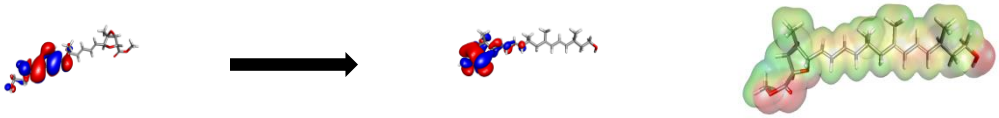
HOMO -6.490949157 (eV) BINDING GAP ENERGY 4.079018098 LUMO -2.411931059 (eV) EPS

FIGURE 5.2.30 CMNPD28966



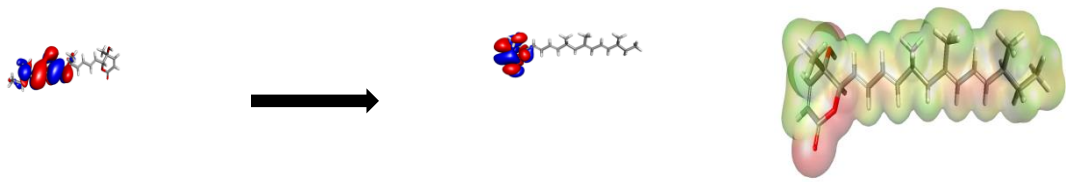
HOMO -6.543180621 (eV) BINDING GAP ENERGY 4.117997883LUMO -2.425182738 (eV) EPS

FIGURE 5.2.31 CMNPD29067



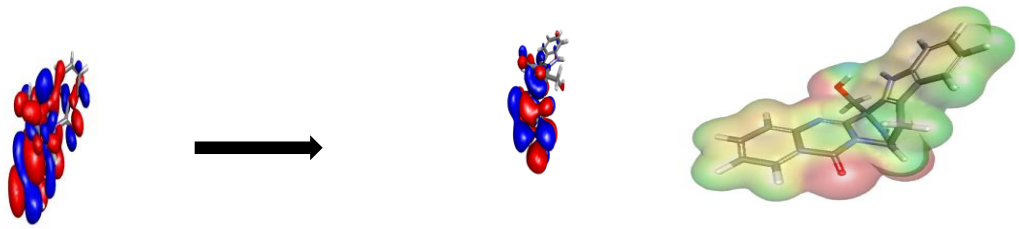
HOMO -5.417925054 (eV) BINDING GAP ENERGY 4.176955461LUMO -1.240969593 (eV) EPS

FIGURE 5.2.32 CMNPD29068



HOMO -5.461853504 (eV) BINDING GAP ENERGY -4.151966145 LUMO -1.309887359 (eV) EPS

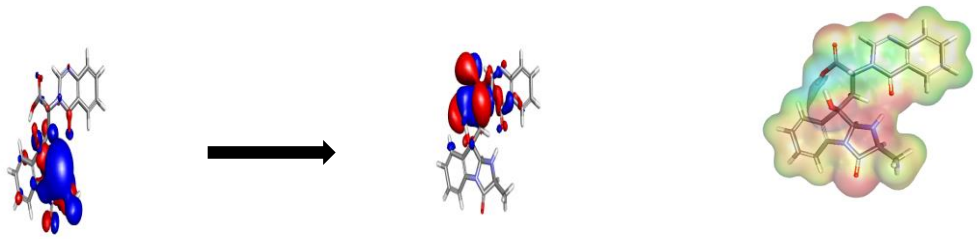
FIGURE 5.2.33 CMNPD29070



HOMO -5.412431889 (eV) BINDING GAP ENERGY 3.582047339 LUMO -1.83038455 (eV) EPS

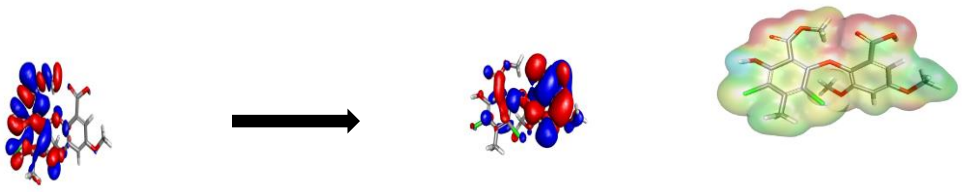
FIGURE 5.2.34 CMNPD30304

/



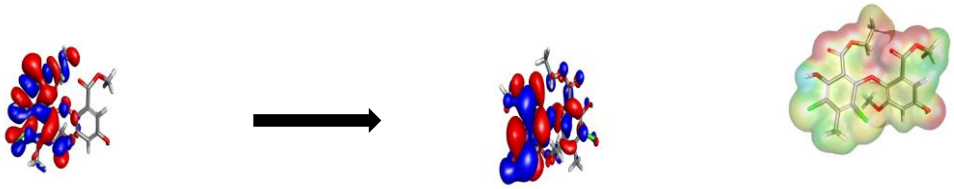
HOMO -5.999289246 (eV) BINDING GAP ENERGY -4.477844145 LUMO -1.521445101 (eV) EPS

FIGURE 5.2. 35 CMNPD30305



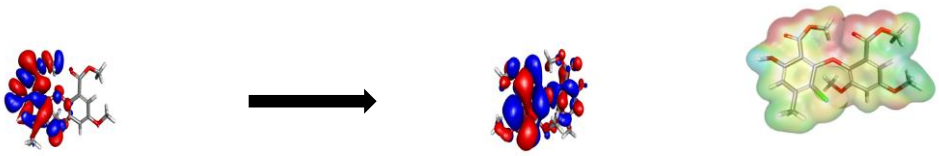
HOMO --6.24751707 (eV) BINDING GAP ENERGY 4.245375258LUMO --2.002141812 (eV) EPS

FIGURE 5.2.36 CMNPD30637



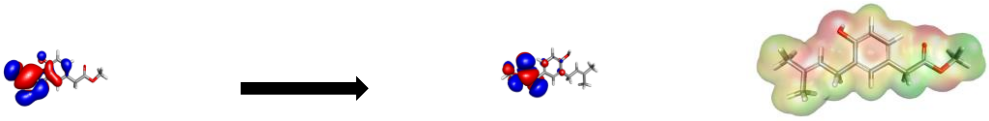
HOMO -6.466045285 (eV) BINDING GAP ENERGY 3.989009865 LUMO -2.477035419 (eV) EPS

FIGURE 5.2.37 CMNPD30638



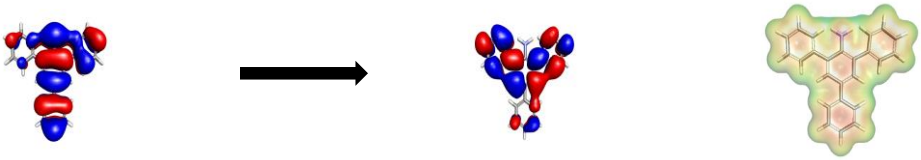
HOMO -6.482700022 (eV) BINDING GAP ENERGY 4.161434351 LUMO -2.321265671 (eV) EPS

FIGURE 5.2.38 CMNPD30639

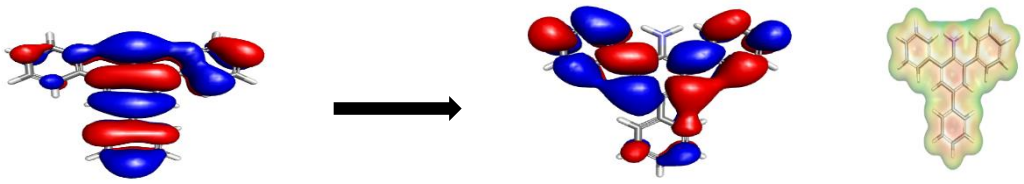


HOMO -6.360022327 (eV) BINDING GAP ENERGY -4.058354306 LUMO -2.301668021 (eV) EPS

FIGURE 5.2.39 CMNPD30643



HOMO -5.642822096 (eV) BINDING GAP ENERGY 5.051910512 LUMO -0.590911584 (eV) EPS

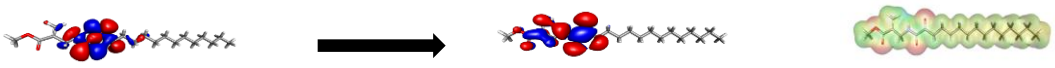


HOMO -4.3999 (eV) BINDING GAP ENERGY -256.206 LUMO -1.6757 (eV) EPS

FIGURE 5.2.40 CMNPD30821

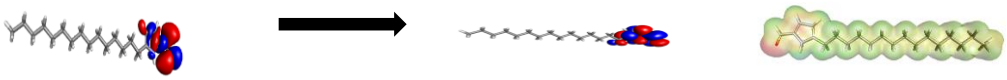
Figure 5.2 dft analysis of marine fungi

MOLECULAR ORBITAL OF SPONGES



HOMO -7.103097061 **(eV)** **BINDING GAP ENERGY** 4.691172533 **LUMO** -2.411924528 **(eV)** **EPS**

FIGURE 5.3.1 CMNPD878

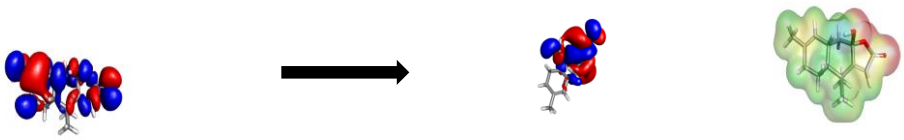


HOMO -6.26598844 **(eV)** **BINDING GAP ENERGY** 4.926395757**LUMO** -1.339592683 **(eV)** **EPS**

FIGURE 5.3.2 CMNPD966

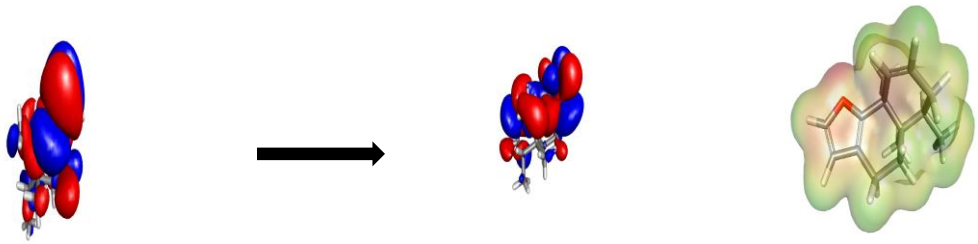
HOMO -6.274699353 **(eV)** **BINDING GAP ENERGY** 4.930106032**LUMO**-1.344593321 **(eV)** **EPS**

FIGURE 5.3.3 CMNPD967



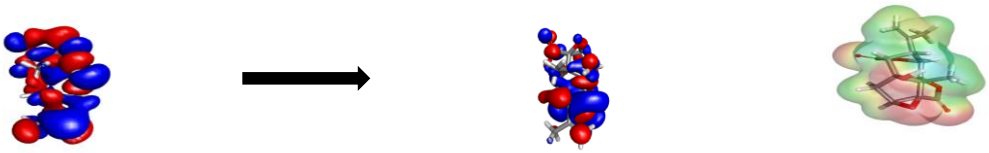
HOMO --6.194366949 **(eV)** **BINDING GAP ENERGY** 4.459726251**LUMO** -1.734640698 **(eV)** **EPS**

FIGURE 5.3.4 CMNPD1065



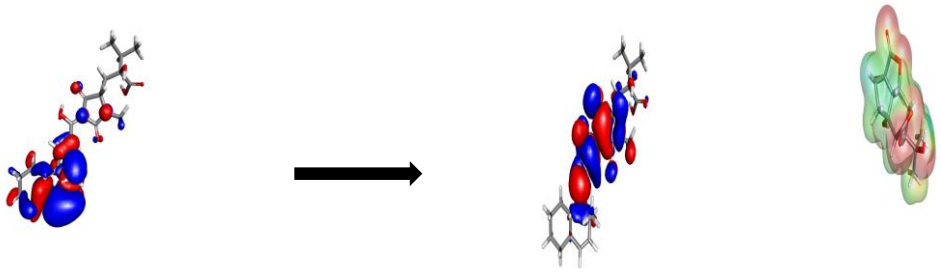
HOMO -5.923252434 **(eV)** **BINDING GAP ENERGY** 6.4983278 **LUMO** 0.5750753661 **(eV)** **EPS**

FIGURE 5.3.5 CMNPD2769



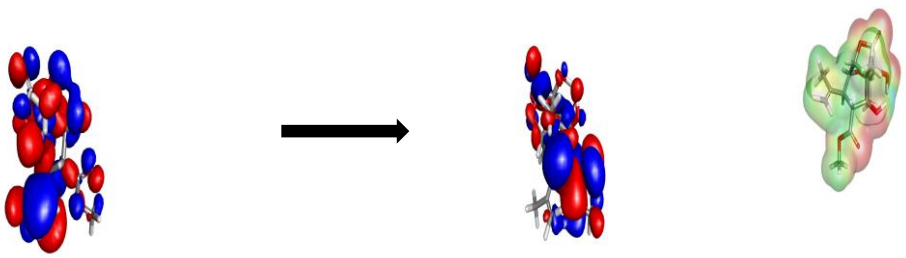
HOMO -6.710569909 **(eV)** **BINDING GAP ENERGY** 5.06896961**LUMO** -1.641600299 **(eV)** **EPS**

FIGURE 5.3.6 CMNPD2771



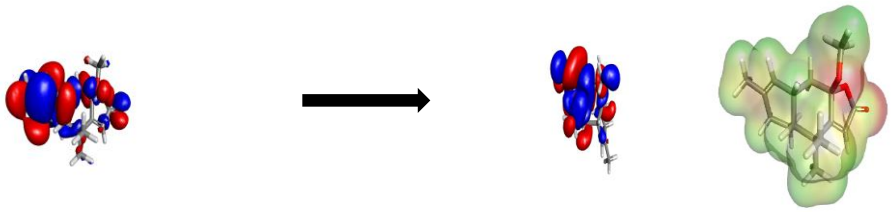
HOMO -7.019430173 **(eV)** **BINDING GAP ENERGY** 5.275861142**LUMO -**-1.74356903 **(eV)** **EPS**

FIGURE 5.3.7 CMNPD2772



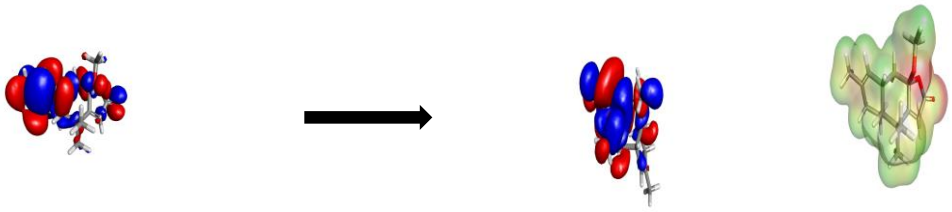
HOMO -6.677358125 **(eV)** **BINDING GAP ENERGY** 5.417211843**LUMO** -1.260146282 **(eV)** **EPS**

FIGURE 5.3.8 CMNPD2773



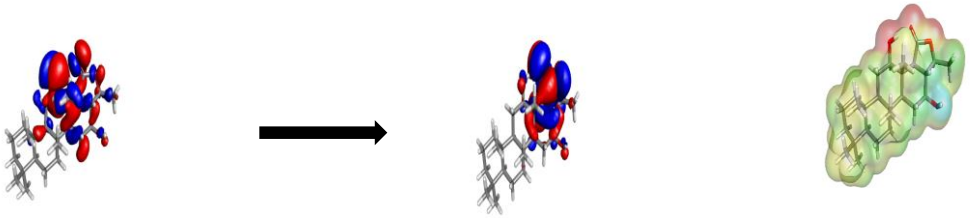
HOMO -6.183380891 **(eV)** **BINDING GAP ENERGY** 4.575246803**LUMO** -1.608134088 **(eV)** **EPS**

FIGURE 5.3.9 CMNPD3038



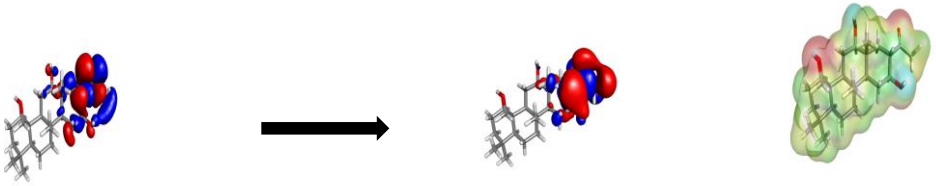
HOMO -6.635640873 **(eV)** **BINDING GAP ENERGY** 5.634800448**LUMO** -1.000840425 **(eV)** **EPS**

FIGURE 5.3.10 CMNPD5010



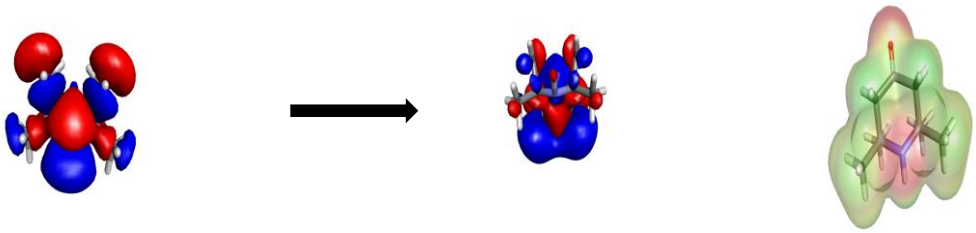
HOMO --6.667926382 **(eV)** **BINDING GAP ENERGY** 5.664769178 **LUMO** -1.003157204 **(eV)** **EPS**

FIGURE 5.3.11 CMNPD5011



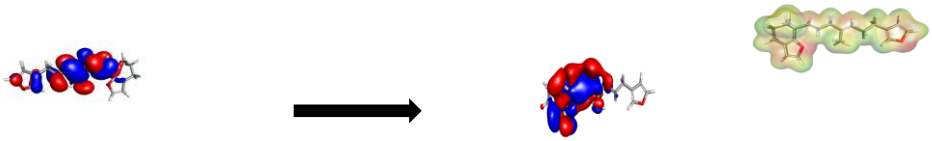
HOMO -6.553890484 **(eV)** **BINDING GAP ENERGY-**5.785377718**LUMO** -0.7685127661 **(eV)** **EPS**

FIGURE 5.3.12 CMNPD5012



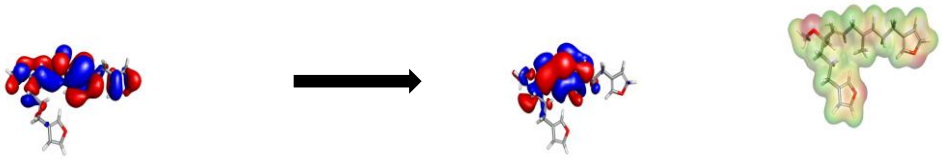
HOMO -4.8642804 (eV) **BINDING GAP ENERGY -134.716904** **LUMO -2.085036 (eV)** **EPS**

FIGURE 5.3.13 CMNPD5149



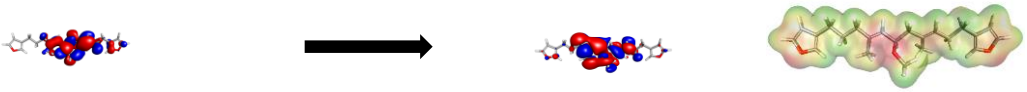
HOMO -4.881520 (eV) **BINDING GAP ENERGY -257.52128** **LUMO -0.409567 (eV)** **EPS**

FIGURE 5.3.14 CMNPD5567



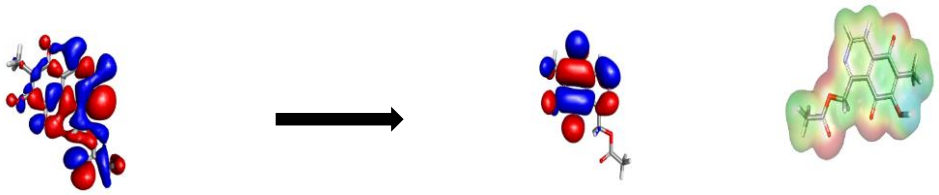
HOMO -5.165386 (eV) **BINDING GAP ENERGY -281.63 89** **LUMO -0.629345 (eV)** **EPS**

FIGURE 5.3.15 CMNPD5568



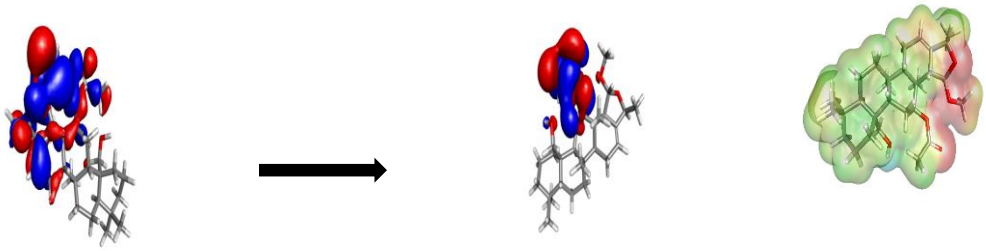
HOMO -5.0813456(eV) **BINDING GAP ENERGY -281.33378** **LUMO -0.486189 (eV)** **EPS**

FIGURE 5.3.16 CMNPD5569



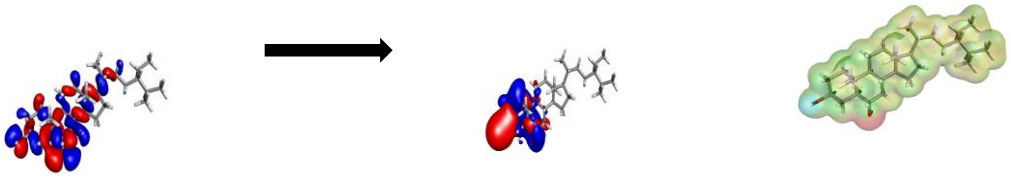
HOMO -5.685434 (eV) BINDING GAP ENERGY -5.6854 567 LUMO -4.4962 789(eV) EPS

FIGURE 5.3.17 CMNPD6139



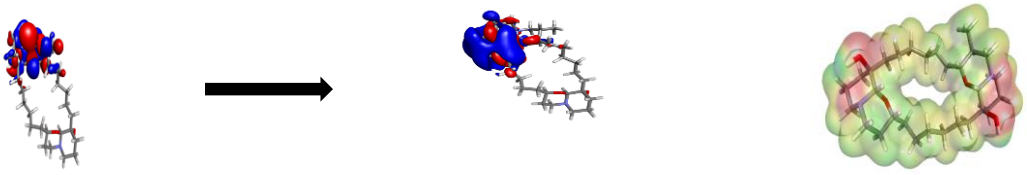
HOMO -6.344337133 **(eV) BINDING GAP ENERGY** 5.989052862 **LUMO -**-0.3552842705 **(eV) EPS**

FIGURE 5.3.18 CMNPD6245



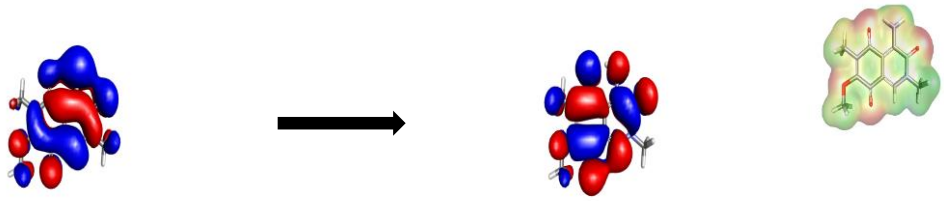
HOMO -5.4502136 (eV) BINDING GAP ENERGY -411.02 567 LUMO -0.1531345 (eV) EPS

FIGURE 5.3.19 CMNPD6261



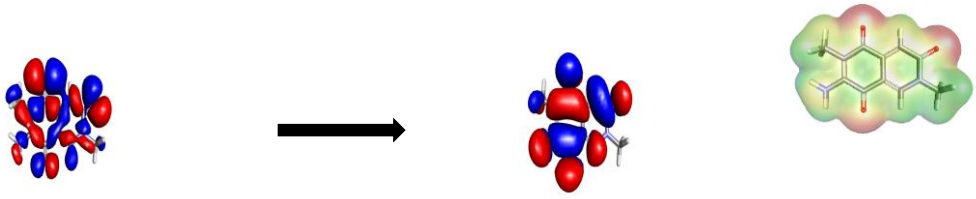
HOMO -6.2535690(eV) BINDING GAP ENERGY -4.25.99356 LUMO 0.6556106 (eV) EPS

FIGURE 5.3.20 CMNPD6716



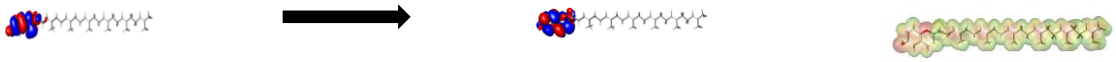
HOMO - -5.308572 (eV) BINDING GAP ENERGY -165.58246 LUMO -3.5667589 (eV) EPS

FIGURE 5.3.21 CMNPD6756



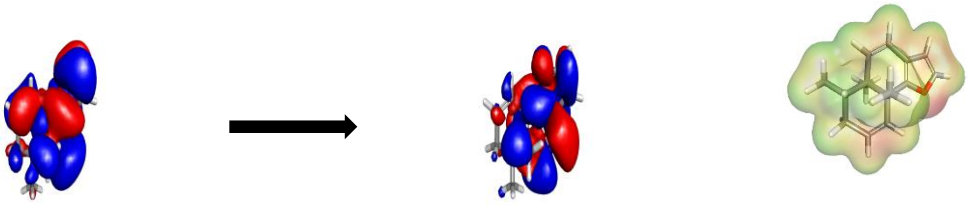
HOMO -5.690805 (eV) BINDING GAP ENERGY -146.5145 LUMO 3.616190 (eV) EPS

FIGURE 5.3.22 CMNPD6757



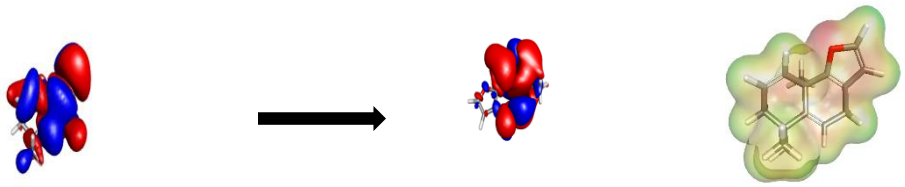
HOMO -5.690547 (eV) BINDING GAP ENERGY -146.51371 LUMO 3.616169 (eV) EPS

FIGURE 5.3.23 CMNPD6872



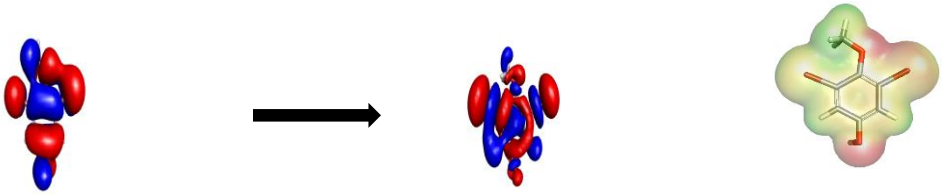
HOMO -4.818047 (eV) BINDING GAP ENERGY -180.92 28 LUMO -1.006958 (eV) EPS

FIGURE 5.3.24 CMNPD6874



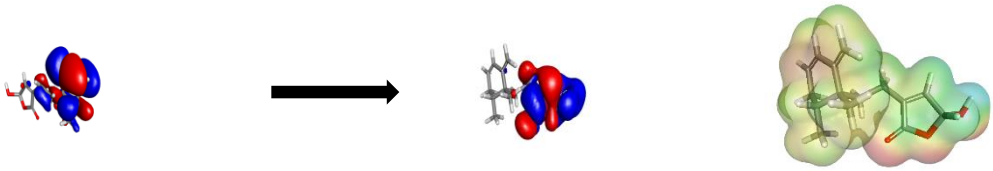
HOMO-5.0773945 (eV) BINDING GAP ENERGY-180.9056 LUMO -0.407808 (eV) EPS

FIGURE 5.3.25 CMNPD6875



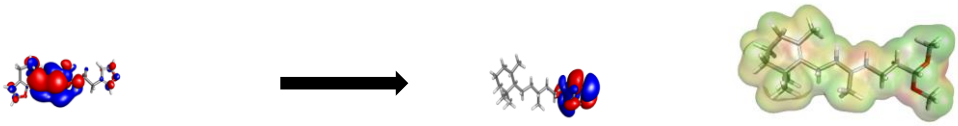
HOMO -5.4485 69(eV) BINDING GAP ENERGY -5.4485456 LUMO -1.748345 (eV) EPS

FIGURE 5.3.26 CMNPD6876



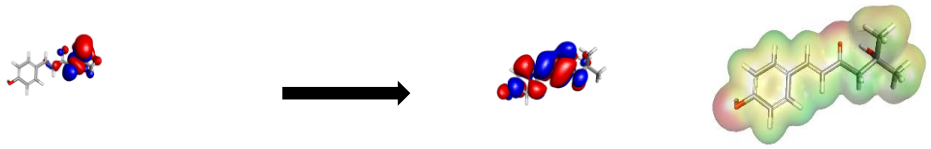
HOMO -5.273994 (eV) BINDING GAP ENERGY -196.69 478 LUMO -2.84119 (eV) EPS

FIGURE 5.3.27 CMNPD6877



HOMO -6.777089 (eV) BINDING GAP ENERGY -266.0 345 LUMO -0.00463347 (eV) EPS

FIGURE 5.3.28 CMNPD6896

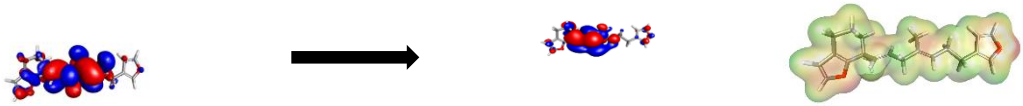


HOMO -5.3086315 (eV) BINDING GAP ENERGY -168.69 3454 LUMO -3.010978 (eV) EPS

FIGURE 5.3.28 CMNPD7623

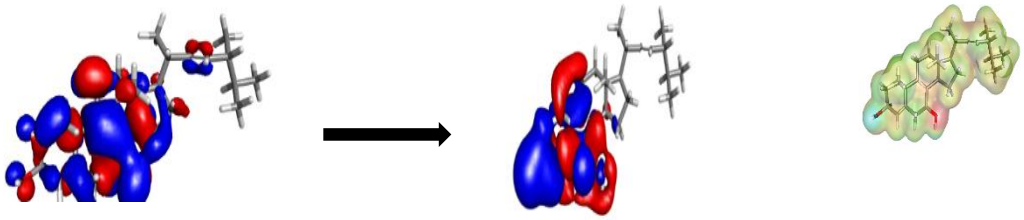
HOMO -5.5300545 (eV) BINDING GAP ENERGY -283.03345 LUMO -0.6576 4(eV) EPS

FIGURE 5.3.29CMNPD7692



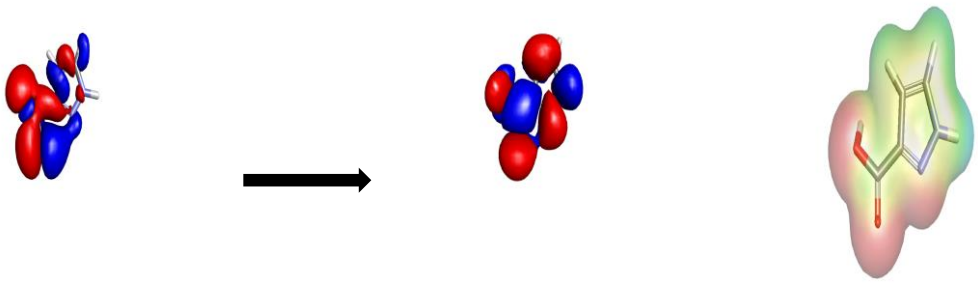
HOMO -5.08734 (eV) BINDING GAP ENERGY -257.50145 LUMO -0.5984 (eV) EPS

FIGURE 5.3.30 CMNPD8324



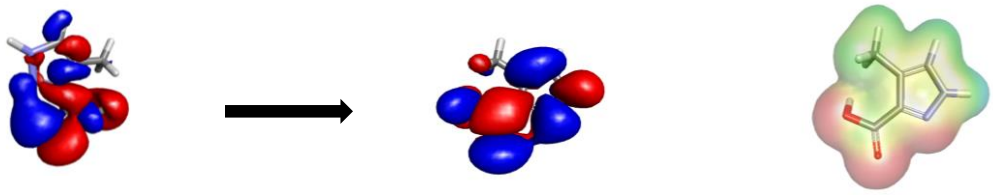
HOMO -5.1466 (eV) BINDING GAP ENERGY -371.39456 LUMO -0.6571 56(eV) EPS

FIGURE 5.3.31 CMNPD8365



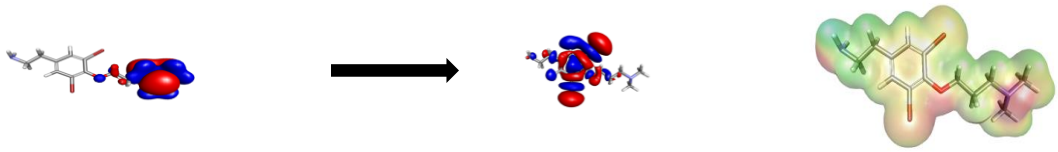
HOMO -6.0691567 (eV) BINDING GAP ENERGY -63.543478 LUMO -2.412789 (eV) EPS

FIGURE 5.3.32 CMNPD8981



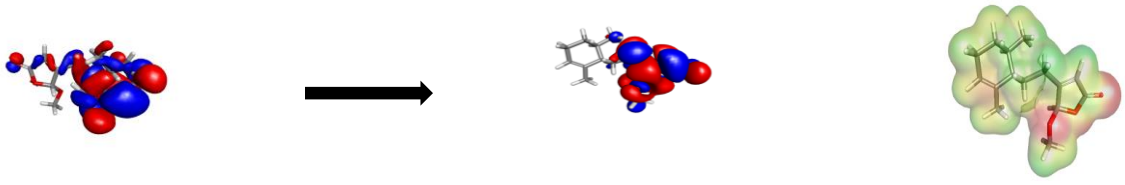
HOMO -6.060085 (eV) BINDING GAP ENERGY 5.279315902 **LUMO -2.352956 (eV) EPS**

FIGURE 5.3.33 CMNPD8982



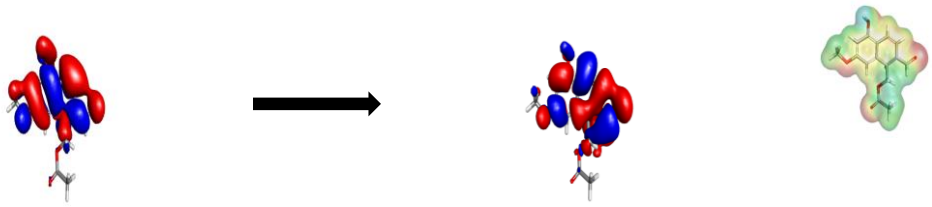
HOMO -4.6285678 (eV) BINDING GAP ENERGY -181.22678 LUMO -1.5688456 (eV) EPS

FIGURE 5.3.34 CMNPD9619



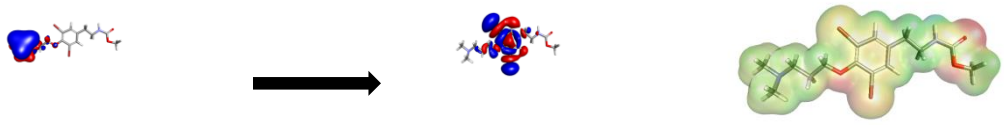
HOMO -5.3532456 (eV) BINDING GAP ENERGY -217.13 678 LUMO -2.5255123 (eV) EPS

FIGURE 5.3.35 CMNPD9738



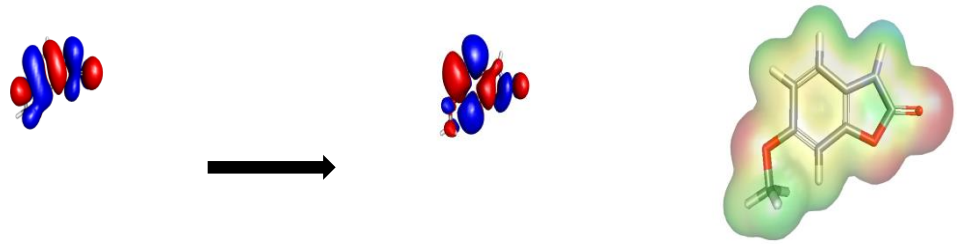
HOMO -4.903145 (eV) BINDING GAP ENERGY -188.74 368 LUMO -1.9404890 (eV) EPS

FIGURE 5.3.35 CMNPD10387



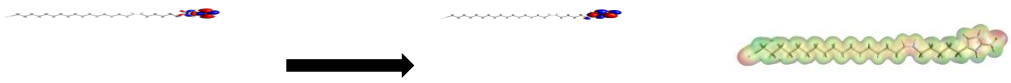
HOMO -4.6694 (eV) BINDING GAP ENERGY -214.3 LUMO -1.7061 (eV) EPS

FIGURE 5.3.36 CMNPD10435



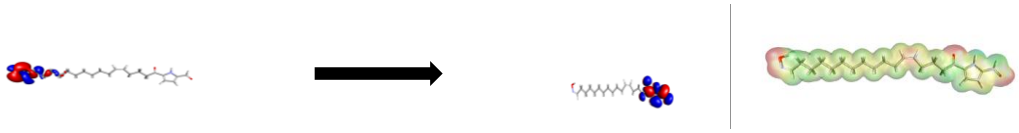
HOMO -5.2582 (eV) BINDING GAP ENERGY -106.24 LUMO -1.317 (eV) EPS

FIGURE 5.3.37 CMNPD10459



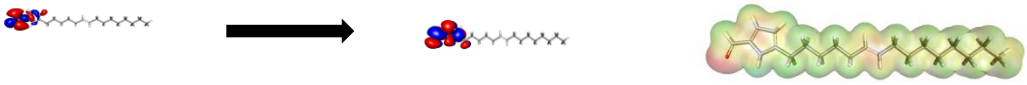
HOMO -5.5616 (eV) BINDING GAP ENERGY -386.7045 LUMO -2.285123 (eV) EPS

FIGURE 5.3.38 CMNPD11117



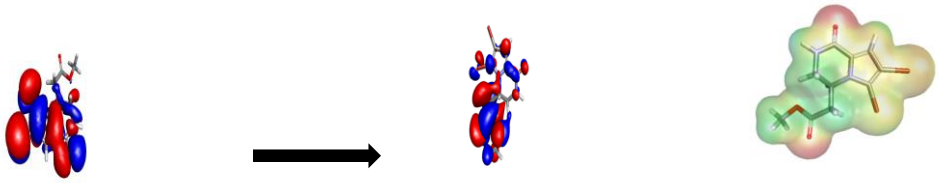
HOMO -6.8320345 (eV) BINDING GAP ENERGY -303.41278 LUMO -3.054 267(eV) EPS

FIGURE 5.3.39CMNPD11118



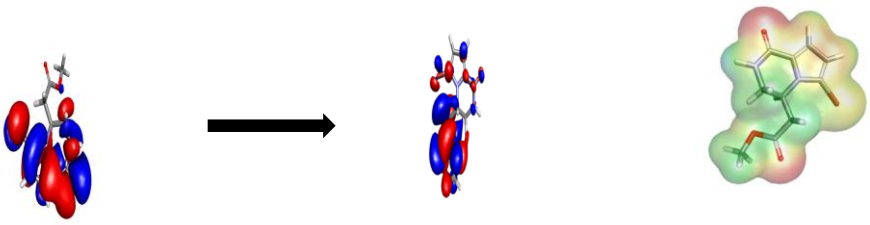
HOMO -5.356123 (eV) BINDING GAP ENERGY -272.3756 LUMO -2.037967 (eV) EPS

FIGURE 5.3.40 CMNPD11119



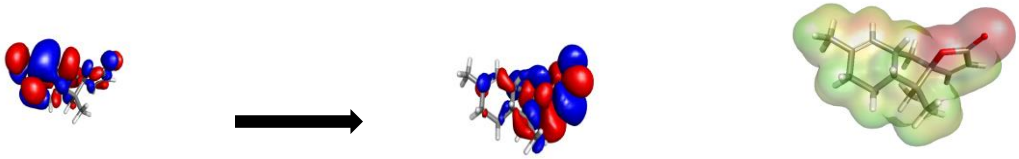
HOMO -5.7218356 (eV) BINDING GAP ENERGY -139.20 345 LUMO -2.236712 (eV) EPS

FIGURE 5.3.41 CMNPD11152



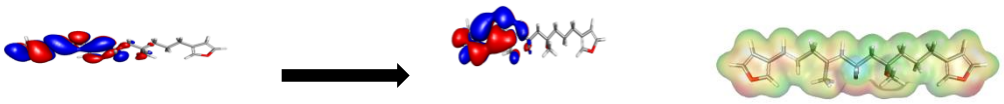
HOMO -6.5765478 (eV) BINDING GAP ENERGY -140.96 247 LUMO -2.1471149 (eV) EPS

FIGURE 5.3.42 CMNPD11153



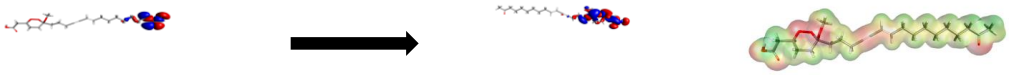
HOMO -5.2918431(eV) BINDING GAP ENERGY -191.28 345 LUMO -2.2714567 (eV) EPS

FIGURE 5.3.43 CMNPD11223



HOMO -4.9507345(eV) BINDING GAP ENERGY -272.42456 LUMO -1.1942890 (eV) EPS

FIGURE 5.3.44 CMNPD11249

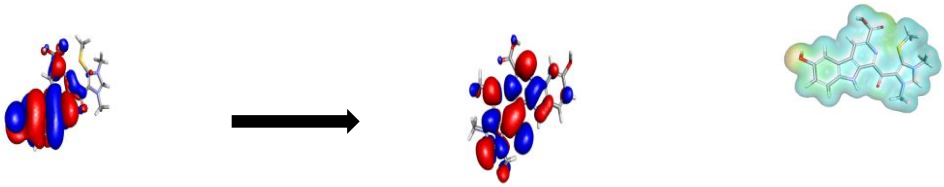


HOMO -5.2958356(eV) BINDING GAP ENERGY -314.15908 LUMO -2.8265456 (eV) EPS

FIGURE 5.3.45 CMNPD11843

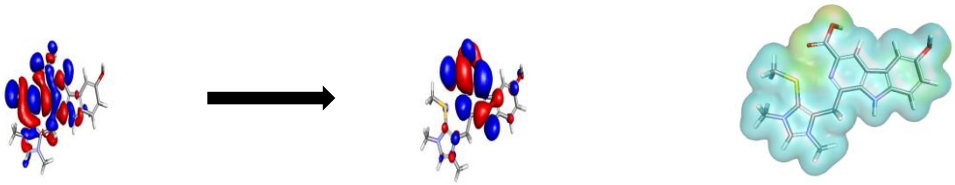
HOMO -5.3581367 (eV) BINDING GAP ENERGY -315.34 135 LUMO -2.537767 (eV) EPS

FIGURE 5.3.46 CMNPD11844



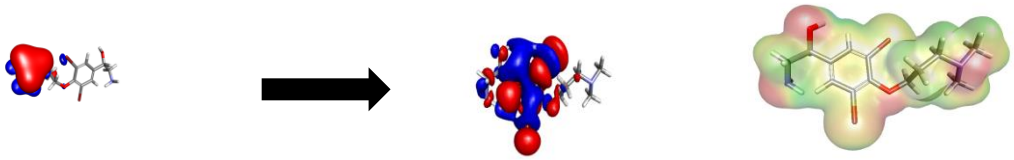
HOMO -6.9626 367(eV) BINDING GAP ENERGY -241.305 146 LUMO -6.5519678 (eV) EPS

FIGURE 5.3.47 CMNPD14212



HOMO -6.7079567 (eV) BINDING GAP ENERGY -242.14 456 LUMO -5.2127678 (eV) EPS

FIGURE 5.3.48 CMNPD14213

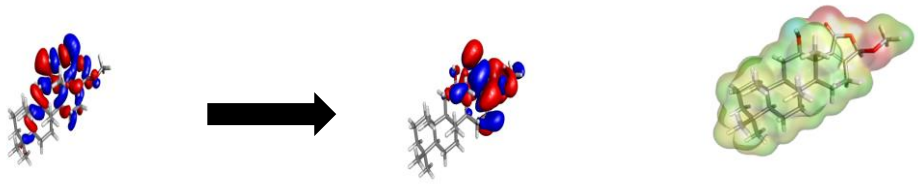


HOMO -6.6014567 (eV) BINDING GAP ENERGY -185.246 345 LUMO -1.939756(eV) EPS

FIGURE 5.3.49 CMNPD14268

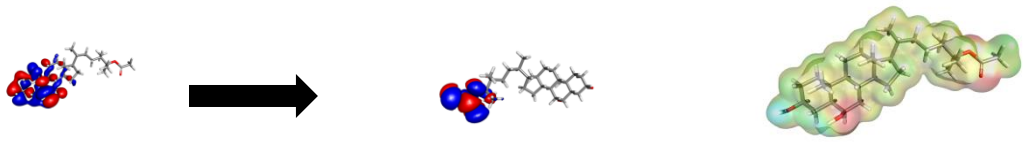
HOMO -199.95345 (eV) BINDING GAP ENERGY -199.95456 LUMO -1.6330 (eV) EPS

FIGURE 5.3.50 CMNPD15143



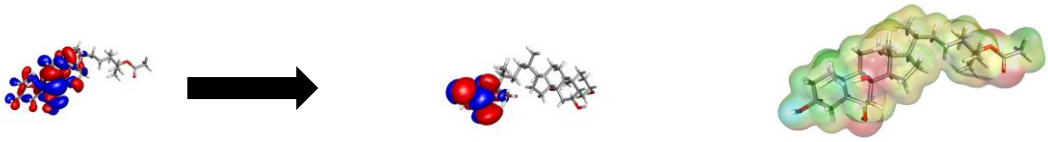
HOMO -4.692345 (eV) BINDING GAP ENERGY -354.72 876 LUMO -2.1556907 (eV) EPS

FIGURE 5.3.51 CMNPD18101



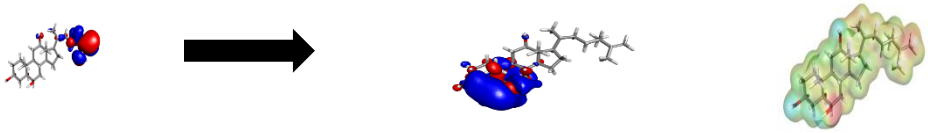
HOMO -5.5462145 (eV) BINDING GAP ENERGY -424.94789 LUMO -1.2562345 (eV) EPS

FIGURE 5.3.52 CMNPD20295



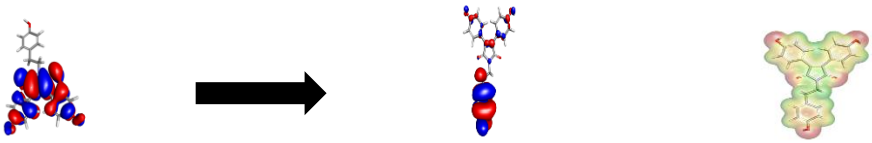
HOMO -5.530923(eV) BINDING GAP ENERGY -426.93 56 LUMO -1.230169(eV) EPS

FIGURE 5.3.53 CMNPD25206



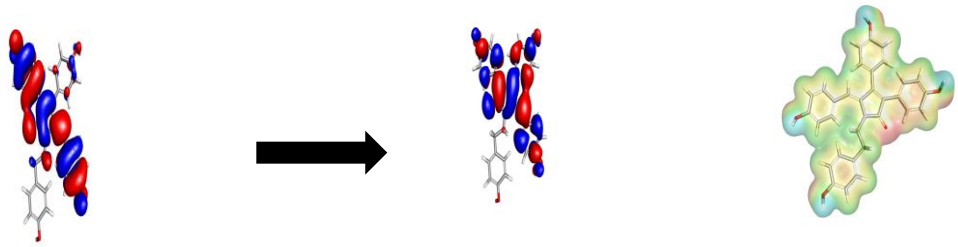
HOMO -5.5644 (eV) BINDING GAP ENERGY -481.3469 LUMO -1.723 458(eV) EPS

FIGURE 5.5.54 CMNPD20297



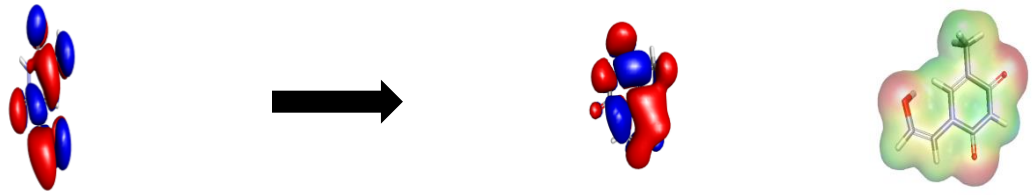
HOMO -6.564490 (eV) BINDING GAP ENERGY -281.34 24 LUMO -3.723367 (eV) EPS

FIGURE 5.3.55 CMNPD25205



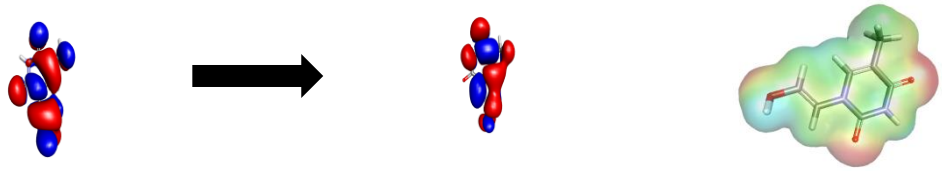
HOMO -5.247956 (eV) BINDING GAP ENERGY -353.84567 LUMO -2.957812 6(eV) EPS

FIGURE 5.3.56 CMNPD25206



HOMO -5.6108567 (eV) BINDING GAP ENERGY -106.35956 LUMO -2.3681456345 (eV) EPS

FIGURE 5.3.57 CMNPD25208

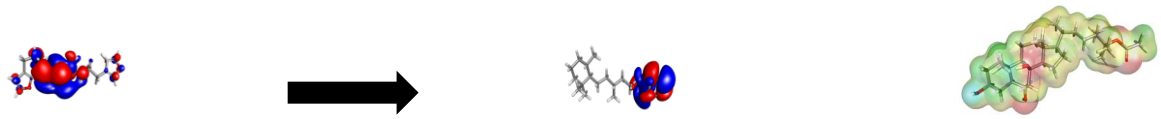


HOMO -5.4877123 (eV) BINDING GAP ENERGY -106.38345 LUMO -2.4496345(eV) EPS

FIGURE 5.3.58 CMNPD25209

HOMO -6.06008 (eV) BINDING GAP ENERGY -1.349087LUMO -2.3529 389(eV) EPS

FIGURE 5.3.59 CMNPD8982



HOMO -5.4485 (eV) BINDING GAP ENERGY -5.4485 LUMO -1.7483 (eV) EPS

FIGURE 5.3.60 CMNPD6876

Figure 5.3 dft analysis of marine sponges

HOMO stands for highest occupied molecular orbital, LUMO stands for lowest unoccupied molecular orbital and EPS stands for electrostatic potential. This shows that charge transfer takes place within the molecule which supports the bioactive property of the molecule. The HOMOs and LUMOs of the dye molecules are displayed which reveals that the HOMO of each dye molecule is localized on the carbon and nitrogen atoms of the porphyrin framework. The LUMOs are also concentrated on the porphyrin framework, with little delocalization.

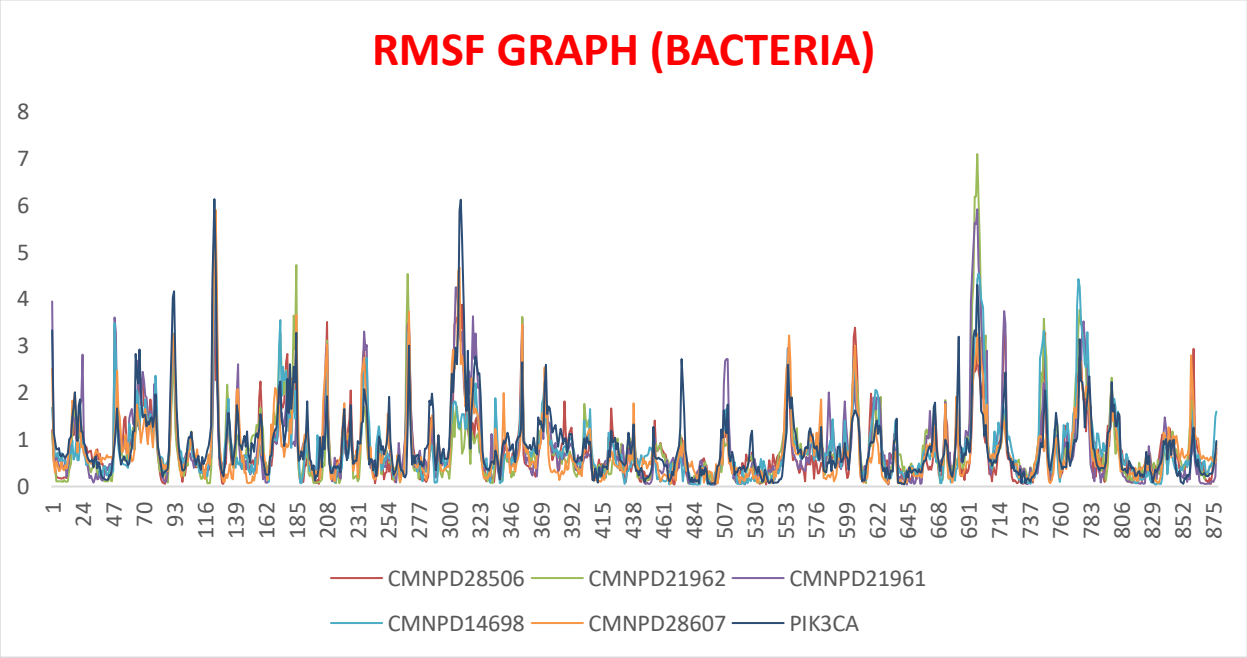


FIGURE 5.4

Simulation graphs, a general language-independent tool for modeling simulation designs, is presented. Simulation graphs are an extension of Petri net graphs. The modifications to ordinary Petri net graphs are explained.

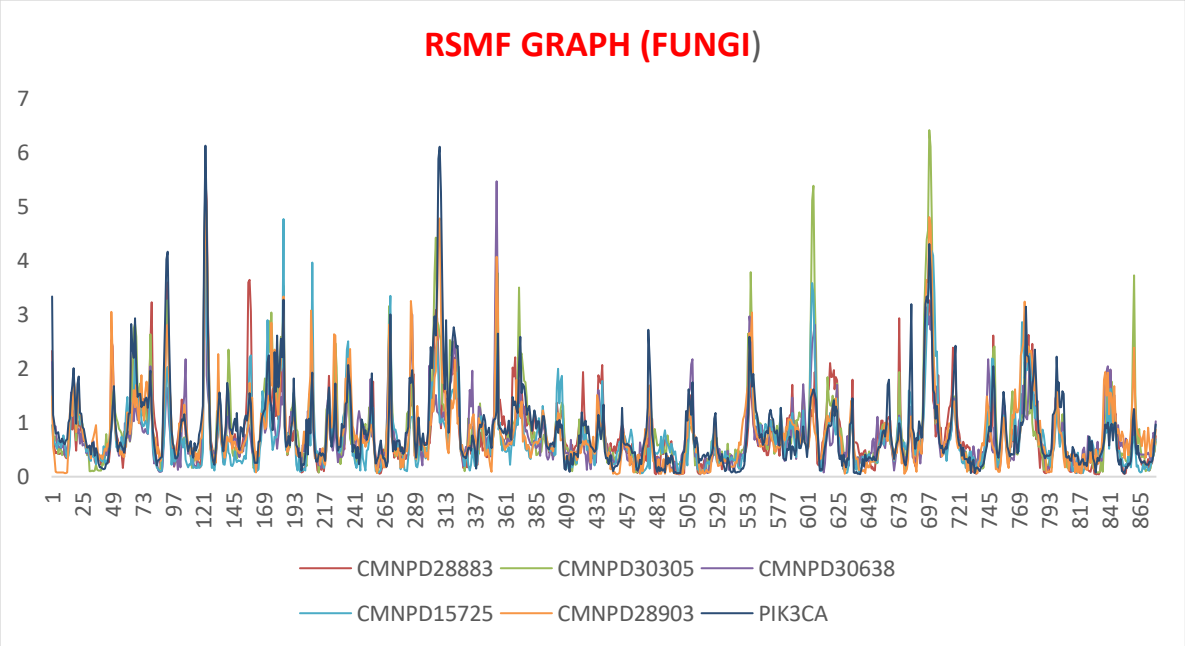


FIGURE5.5

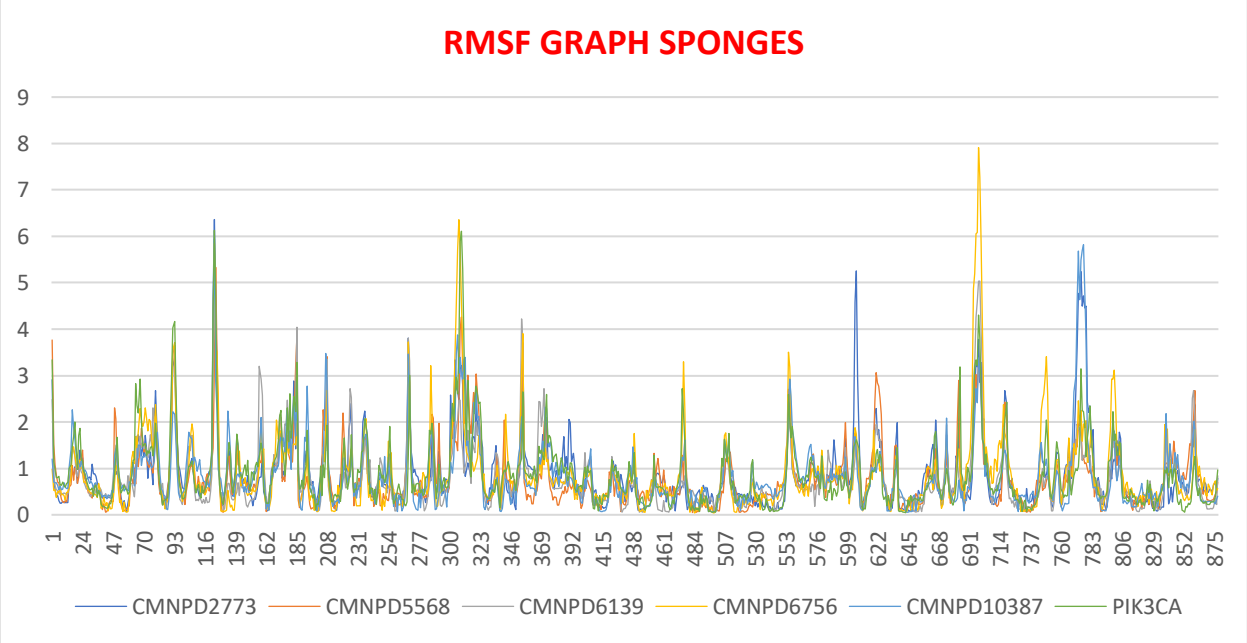


FIGURE 5.6

Simulation graphs, a general language-independent tool for modeling simulation designs, is presented. Simulation graphs are an extension of Petri net graphs. The modifications to ordinary Petri net graphs are explained.

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