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Structure-activity relationship of a bioactive compound in Ocimum gratissimum

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ABSTRACT:As the use of medicinal plants to treat diseases gain wider acceptance, it becomes necessary to continue to research on the structures of their bioactive components and the structure-activity relationships between the compounds and the diseases they treat.Bioactive compounds in Ocimum gratissimum was studied by extracting it with 99% ethanol. After which it was chromatographically fractionated into three fractions with chloroform, ethyl acetate and n-hexane using a silica gel column. Gas chromatography – mass spectrometry wasused to determine the library identities of the extracts. Comparisons were made between the structures found in the samples and the diseases they are used to treat locally. Ocimim gratissimum has been used widely as an antioxidant. It was discovered that 2-isopropyl-5-methylphenol was the compound responsible for the antioxidant properties of Ocimim gratissimum. The presence of 2-isopropyl-5-methylphenol, an antioxidant contributes greatly to its medicinal qualities by acting as a free radical scavenger made possible by the inductive effect of the ortho isopropyl group and the conjugation of the benzene ring

KEYWORDS: Ocimim gratissimum, Antioxidant, 2-isopropyl-5-methylphenol

I. INTRODUCTION

Medicinal plants are sources of bioactive compounds used in the treatment of different types of diseases. Synthetic drugs are usually drugs produced in the laboratory using chemical precursors, following specific, synthetic pathways. After the synthesis such drugs are formulated in various ways such as pills, syrups, capsules, balms, infusions, drops and so on. The chemistry of drug discovery normally start with the isolation and purification of the bioactive compounds of a known medicinal plant by solvent extraction and chromatography [1, 2]. After which the structure of the active principle is determined using various spectroscopic methods such as gas chromatography-mass spectrometry, Fourier transform infrared spectroscopy, and nuclear magnetic resonance spectroscopy.

Among the numerous natural plant products used in the herbal treatment of diseases is Ocimungratissimun,. This research aims at spectroscopically determining the structures of their active components and the relationships between such structures and the diseases they cure [3]. Structure–activity relationship is the connection between a compound and its biological activity. Determination of structure–activity relationship facilitates the analysis of the chemical groups responsible for inducing a target biological action in an organism.

A pharmacophore is the collaboration of steric and electronic features that is required to certify the optimal supramolecular interactions with a particular biological target in order to activate or hinder its biological response [4]. In recent times pharmacophore modelling is a vital ligand-based approach used in drug discovery. It is a term that describes the configurations of chemical features that are common to all of the ligands.

A pharmacophore hypothesis assembles the collective features in the three-dimensional space representing groups in a molecule that contribute in significant interactions between the drug and the active site [5].

II. EXPERIMENTAL

500 grams of Ocimungratissimunleaf was washed with distilled water and dried in an oven at the temperature of 50^{O}C for 5hours. The dried

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samples was then crushed with mortar and pestle to powdery form and soaked in 1000mLs of 96% ethanol in a plastic container and covered. The mixture was agitated hourly for 3days after which it was filtered using muslin cloth followed by filtration by whatman No 1 filter paper. The extract was heated in a water bath to evaporate the ethanol and recover the crude extract [6]. The slide for thin layer chromatography was prepared by mixing silica gel and ethanol using mortar and pestle and poured on two glass slides. The slides was dried in an oven at 80^{O}C. The crude extract was dropped on the thin layer chromatography slide and dipped into the beaker containing the mixture of N-Hexane, chloroform and ethyl-acetate with the side containing the drop of crude extract above the reagent. The second slide with the drop of the sample crude extract was dipped into a beaker containing a mixture of n-Hexane and chloroform. Silica gel, crude extract of the sample and N-Hexane was mixed together in a mortar with pestle.

The mixture was then dried in an oven at 63^{O}C. The column burette was clamped to a retort stand. The prepared dried sample powder was filled into the column burette and connected to a vacuum pump. The N-Hexane was poured into the burette and the N-Hexane fraction collected in a conical flask. Afterwards chloroform was poured into the sample in the column burette and the chloroform fraction collected in another conical flask. Lastly, the ethyl-acetate was poured and the ethyl-acetate fraction was also collected in a separate conical flask [7]. The eluates were separately concentrated in a rotary evaporator connected to the vacuum pump at temperature of 70^{O}C.The eluates were subjected to GC-MS analysis.

III. RESULTS AND DISCUSSION

Table 1 Table 1: Library IDs of the GC-MS analysis of OcimimgratissimumLeaf Extract

2-isopropyl-5-methylphenol
n-Hexadecanoic acid
Phytol
(Z,Z,Z)-9,12,15-Octadecatrienoic acid
Butyl citrate
1,4-Benzenedicarboxylic acid
Phthalic acid
Methyl 8,11,14,17-eicosatetraenoate

Thymol (2-isopropyl-5-methylphenol) is one of the major bioactive compounds found in the GCMS library ID of the extracts from Ocimim gratissimum.The leaves of Ocimim gratissimum has been used as anti-inflammatory agent for the treatment of upper respiratory tract infections. The presence of 2-isopropyl-5-methylphenol, an antioxidant contributes greatly to its medicinal qualities. What is the relationship between 2-isopropyl-5-methylphenol and its ability to eliminate free radicals from biological systems? The 2-isopropyl-5-methylphenol is ionized, to a phenoxide ion which in turn transfers one electron to a free radical, neutralizing it as is shown in the following reactions [8].

The normal functioning of organs in biological systems constantly generate free radicals which cause oxidative stress and damage the DNA, RNA and organ proteins which leads to aging, inflammation and immunosuppression. Antioxidants such as thymol (2-isopropyl-5-methylphenol) can help reduce the effect of the free radicals by scavenging them out of biological systems. The inductive effect of the ortho isopropyl group and the conjugation of the benzene ring makes it a very good free radical scavenger [9].

IV. CONCLUSION

The use of natural plant extracts to treat diseases is gaining increasing popularity world over. Most persons who administer such medicinal plants as drugs have little knowledge of the structures of their bioactive components. Also little research has been carried out on the structure-activity relationships between the compounds in most local medicinal plants and the diseases they treat. Once the structure of the active compound is known, medicinal chemists try to determine the structure-activity relationships between the drugs and the diseases they are used to cure. Knowledge of such structure-activity relationships will aid in the discovery of the pharmacophore of the compound which will in turn facilitate synthesis of the analogues of such drugs[4].

The design and synthesis of novel drug structures are carried out to increase activity, to reduce side-effects, and to provide easy and efficient methods of administration. The structural modifications used to improve the quality of the synthesized drug include: variation of substituents, extension of the structure, chain extensions or contractions, ring expansions or contractions, ring variations, simplification of the structure and rigidification of the structure. All these activities are carried out to improve the quality of the initial natural, medicinal plant. In addition, some researchers argue that natural herbal drugs have fewer side effects and strengthens the immune system, besides being cheaper to obtain and more available.

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