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The Synthesis, Isolated and Characterization Conjugated Linoleic Acid (CLA) From Datura Innoxia Mill Seed

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ABSTRACT

The identification of conjugated linoleic acid (CLA) in Datura species represents a novel and promising avenue for biomedical exploration. CLA comprises a group of positional and geometric isomers of linoleic acid, renowned for their wide-ranging health benefits, including anti-obesity, anti-diabetogenic, and anti-carcinogenic properties. While CLA is conventionally obtained from ruminant-derived dairy and meat products, the discovery of its potential occurrence in Datura offers a compelling plant-based alternative source. Preclinical studies have established CLA's ability to inhibit tumorigenesis via multiple mechanisms, including the induction of apoptosis, suppression of cell proliferation, modulation of immune responses, and inhibition of angiogenesis. However, clinical trials in human subjects have yielded inconsistent outcomes, highlighting the need for continued investigation into its efficacy and therapeutic scope. Building upon these insights, the present study aims to extract, purify, and characterize CLA from Datura seeds, followed by evaluation of its anticancer potential. This will involve in vitro cytotoxicity assays against human cancer cell lines and mechanistic studies to elucidate its molecular mode of action. The overarching goal is to develop a CLA-based natural formulation with potential application as an anticancer therapeutic agent

KEY WORD: Datura Innoxia Mill, CLA, Reflex reaction, Magnetic steroid,

INTRODUCTION

Datura is a wild weed belonging to family Solanaceae, its name derived from Sanskrit word "Dhutra" (divine inebriation) is used for its healing properties. Various species of Datura are known and widely employed for their medicinal and toxic properties that are based upon more than 30 alkaloids. Because of their funnel form, fragrant nocturnal blooms, species such as Datura inoxia, Datura metel, Datura stramonium and Datura wrightii are cultivated as ornamental plants with all but D. metel known from wild populations (DeWolf, 1956). Navajos chewed dried roots to reduce fever. Zunis made poultice from it to treat inflammation and bruises (Del Pozo, 1966). In China, it is known as "Yangjinhua" and used for the treatment of asthma, convulsions, pain, and rheumatism (Pan et al., 2007). Flos Daturae has an effect on the treatment of psoriasis for clinical use in China (Guarrera, 1999). It is used in Italy to remove lice from hen bundles. D. innoxia Mill seeds are used for acne and bronchitis in Sakarya province of North-west Turkey and locally called "Tatala", while the petroleum ether extract is also found to possess antimicrobial activities against Esherichia coli and Trachystemon orientalis by Uzun et al. (2004). It is also used commonly in ethno veterinary practices in Nepal (Raut and Shreshtha, 2012) and by Gujjar community in India (Gaur et al., 2010). In Ayurveda, Datura plant parts are used to treat various disorders including asthma, skin disorders, jaundice, piles, and diabetes (Dash and Kashyap, 1991). Datura seeds have been used as a prophylactic measure to treat

animal bites, especially dog bites. Person bitten by mad dog is administered with juice of Datura along with butter milk and jaggery. Also, the site of bite is smeared with a paste of the fruit (Papadoyannis, 1995). Extensive research has been carried out since 1925 for the isolation and characterization of the total alkaloid contents in Datura species (Berkov et al., 2006; Dovelana et al., 2006). Vitale et al. (1995) has shown that the total alkaloid content in Datura varies from 0.02 to 0.52% and scopolamine from 0.0029 to 0.32% relative to the dried material, depending on the geographical area, the part of the plant studied and the stage of growth[1].

Natural product chemistry is one of the most remarkable fields of study on health sciences; it is usually regarded by the layman as one of the most abstruse and remote from everyday life and thought. The term natural product is commonly reserved for those organic compounds of natural origin that are unique to one organism, or common to a small number of closely related organisms. The term secondary metabolite is typically used to refer to an organic compound of limited distribution in nature (Williams & Lemke, 2002). The study of natural products has had a number of rewards. It has led to the discovery of a variety of useful drugs for the treatment of diverse ailments and contributed to the development of separation science and technology, spectroscopic methods of structure elucidation and synthetic methodologies that now make up the basics of analytical organic chemistry (Taura et al., 2014). Herbal remedies have been used for centuries but more recently the compounds that are active have been identified and this has enabled them to be extracted and purified.

Figure 1 – Datura Innoxia Mill

Synthetic organic chemists have then been able to produce the molecules in vitro and so produce them on larger scales.[2]

Datura mainly contains the tropane alkaloids atropine, scopolamine, and hyoscyamine. Uses of datura have long histories of hallucinogenic use and have been connected with sorcery, witchcraft, native medicine, and magico-religious rites dating back to 1500 BC and Homer's Odyssey. (Homer's use of the plant moly as an antidote to Circe's poisonous anticholinergic drugs may have been the first recorded use of an anticholinesterase to reverse central anticholinergic intoxication). Chinese herbal medicines containing tropane alkaloids have been used to treat asthma, chronic bronchitis, pain, and flu symptoms. In Mexico, Datura is taken by Yaqui women to lessen pain of childbirth. In Africa, a common use is to smoke leaves from Datura to relieve asthma and pulmonary problems. Many cultures worldwide add plants with tropane alkaloids (particularly Datura species) to alcoholic beverages to increase intoxication. Recently, Datura has been used as a recreational hallucinogen in the US, resulting in sporadic cases of anticholinergic poisoning and death[3].

Datura innoxia Mill., a lesser-studied species within the Datura genus, has received limited scientific attention regarding its phytochemical profile and therapeutic potential. In the present study, we aimed to identify and analyze the bioactive chemical constituents present in the fruit of Datura innoxia. Preliminary investigations have revealed the presence of several biologically active compounds with potential pharmacological relevance.

The primary objective of this research is to explore the chemical composition of Datura innoxia Mill with a focus on isolating compounds that may serve as candidates for anticancer drug development. By identifying and characterizing these compounds, we aim to lay the groundwork for the formulation of a novel anticancer agent derived from Datura innoxia Mill.

METHODS AND MATERIAL

Collection of Material: We collected a sample of Datura from the ground area of Bakori Phata in Wagholi. We prepared a herbarium specimen of this Datura plant and obtained an identification & Authentication certificate from BSI Pune, which identified its species as Datura innoxia Mill.

Botanical Description of Datura innoxia Mill: Datura innoxia Mill., commonly known as pricklyburr, downy thorn-apple, or sacred datura, is an herbaceous annual or short-lived perennial belonging to the Solanaceae (nightshade) family. Habit: Typically grows as an erect or spreading, bushy herb, reaching heights of 0.3 to 1.5 meters and can spread up to 2 meters in diameter. Stem: The stems are smooth, often purplish, and covered with dense, short, grayish hairs (pubescent), sometimes glandular. Leaves: The leaves are simple, alternate, and supported by long stalks (petioles). The leaf blade is typically ovate to elliptic, 5-18 cm long and 4-15 cm wide, with an asymmetric, broadly wedge-shaped to truncate base and an acute apex. The margins are usually entire or irregularly toothed and both surfaces are covered in fine, grayish hairs. Crushed leaves emit an unpleasant odor. Flowers: The flowers are solitary, large (12-19 cm long), and trumpet-shaped (tubular) with a white or creamy corolla, sometimes tinged with purple. They are erect initially and may become nodding later. The calyx is long and tube-like (8-10 cm). They have a pleasant fragrance, especially at night. Fruit: The fruit is a nodding, globose to ovoid capsule, about 3-5 cm in diameter, densely covered with slender, soft spines. It is initially purple-green to brownish when ripe and splits open irregularly at the apex to release numerous black seeds (4-5 mm long). Roots: May develop a tuberous root system.

Materials and chemicals: Round bottom flask,, rota evaporator, digital measuring balance, Heating Mantle, Beaker, conical flask, Condensers, Funnel, Glass Road, Whatmean filter paper, Thin layer chromatography (TLC) plate (precoated aluminum sheet, 20 x 20 cm), UV-Spectrometer, FTIR, H-NMR, C-NMR, GC-MS, Water, Acetone, Petroleum ether, n-Hexane, Ethyl acetate, Ethanol (95%), DMSO. All characterization test are obtained from department of chemistry SPPU pune.

Methods:

Seed Preparation and Extraction: Datura seeds were separated from mature fruits and thoroughly dried under ambient conditions. The dried seeds (100 g) were finely ground using a mortar and pestle. The resulting powder was transferred to a 1 L round-bottom flask containing 500 mL of distilled water. The mixture was subjected to reflux for 3.5 hours. After cooling, the setup was allowed to stand overnight. On the following day, the mixture was again refluxed for an additional 3.5 hours. Upon completion, an oily layer formed on the surface of the aqueous phase. This oil layer was carefully separated and collected for further use.

Reaction with Hydrobromic Acid: A 20 mL portion of the extracted oil was mixed with 100 mL of aqueous hydrobromic acid (HBr) in a 200 mL beaker. The mixture was stirred continuously using a magnetic stirrer for 5 hours at room temperature. Following the reaction, a white, sticky paste formed, which was isolated as the product.

Figure 2 – Reflex Reaction

Figure 3 – Oily Layer

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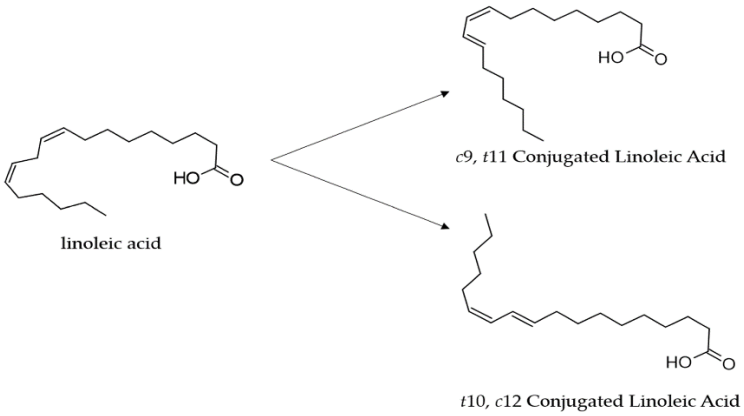
Figure 3 – Product



RESULT AND DISCUSSION:

1. TLC

The Purity of the product is checked with the help of TLC by using coated aluminium foil. The product is loaded by preparation of solution in DMSO. The loaded TLC allowed to run in solvent n-hexane (7) : ethyl acetate (3). Rf values is then calculated.

Figure 4: TLC Plate product

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Rf = Distance travelled Product / Distance travelled by Solvent

= 2/7

= 0.740

2. IR SPECTRA

The Solid Infrared spectral study were done by BRUKER FTIR Instruments from Department of Chemistry, SPPU Pune in the range 500 cm-1 to 3500 cm-1 range.

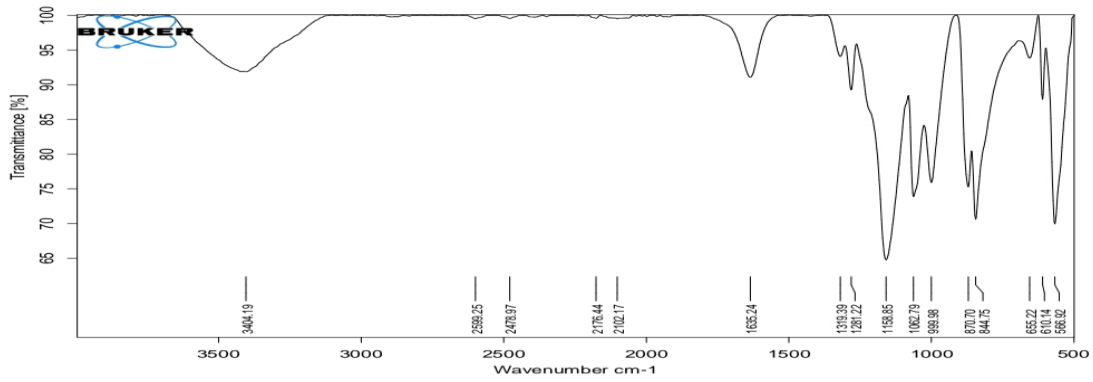

Figure 5 : IR Spectra product

3404.19cm-^{1}	O-H	Alcohol group OH
1635.24cm-^{1}	C=O	Carbonyl group
1319.39cm-^{1} 1281.22cm-^{1}	C-O	C-O-C C=O-O-R
1062.79cm-^{1} 999.98cm-^{1}	C-O	Alcohol group OH Ether group C-O-C
870.70cm-^{1} 844.75cm-^{1}	C-H	Aromatic ring Alken group

Table 1 : IR Spectral values of Product

3. H^{1}-NMR SPECTRA

The H^{1}-NMR SPECTRA study were done by BRUKER Instruments from Department of Chemistry, SPPU Pune in the range 0 to 15 ppm range.

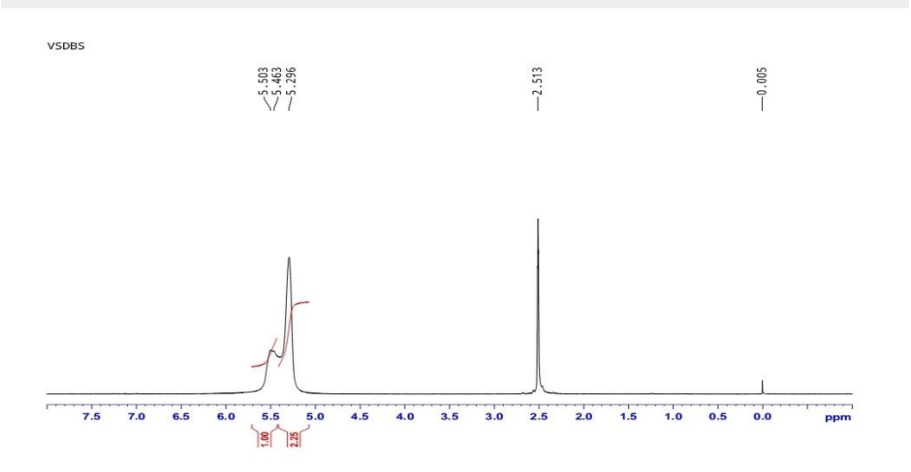

Figure 6 : H1NMR Spectra product

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5.503ppm	C=C	I I R-C=C-H
5.463ppm	Alkene protons	
5.296ppm	Alkene protons	
2.513ppm	C=0	O II I RO-C-C-H I
0.005ppm	This peak is likely from a solvent residual peak.	

Table 2 : H-NMR Spectral values of Product.

4. GC-MS SPECTRA

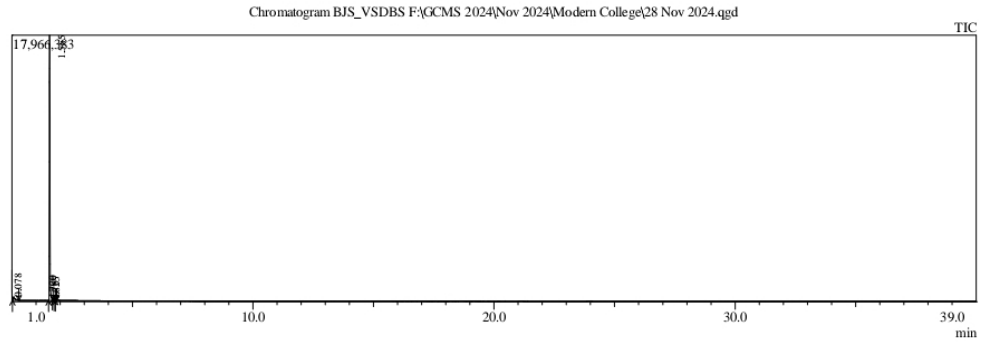
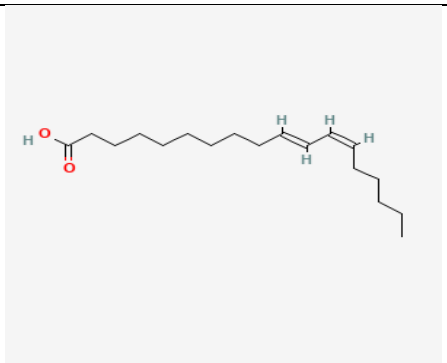


Figure 7 : GC-MS Spectra product

Determining the molecular and structural formula of a compound using Infrared (IR) spectroscopy, Proton Nuclear Magnetic Resonance (^1H NMR) spectroscopy, Carbon-13 Nuclear Magnetic Resonance (^13C NMR) spectroscopy, and Gas Chromatography-Mass Spectrometry (GC-MS) involves a systematic approach

Name	IUPAC Name	Molecular formula	Structural formula
CLA (Conjugated Linoleic acid)	(10E,12Z)-octadeca-10,12-dienoic acid	$C_{18}H_{30}O_2$	

The identification of conjugated linoleic acid (CLA) in Datura species presents a promising avenue for biomedical research. CLA is a group of positional and geometric isomers of linoleic acid, known for its diverse health-promoting properties, including anti-obesity, anti-diabetogenic, and anti-carcinogenic effects. Although CLA is traditionally sourced from ruminant-derived dairy and meat products, the potential presence of CLA in Datura suggests an alternative plant-based source worth investigating.

Preclinical studies have demonstrated CLA's capacity to suppress tumorigenesis through mechanisms such as induction of apoptosis, inhibition of cell proliferation, modulation of immune responses, and interference with angiogenesis. Despite encouraging results in animal and in vitro models, clinical trials in humans have shown variable outcomes, indicating that further research is necessary to clarify CLA's efficacy and therapeutic window in cancer prevention and treatment.Building on these findings, our forthcoming research will focus on the extraction, purification, and characterization of CLA from

Datura seeds, followed by evaluation of its anticancer activity. This will include in vitro cytotoxicity assays against human cancer cell lines and mechanistic studies to elucidate its mode of action. The ultimate objective is to develop a CLA-based formulation with potential application as a natural anticancer therapeutic

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