جـــامـعـة الـــشـرق الأوسـط
MIDDLE EAST UNIVERSITY
Amman - Jordan

Evaluation of the Inhibitory Effects of Polyphenols from Elettaria cardamomum Extract on Staphylococcus aureus, Collagenase, and Tyrosinase: In Vitro Investigations for pharmaceutical FormulationPrepared

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تقييم التأثيرات المثبطة للبوليفينولات من مستخلص الهيل على المكورات العنقودية الذهبية والكولاجيناز والتيروزيناز: دراسات مخبرية

إعداد

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إشراف

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قُدمت هذه الرسالة استكمالاً لمتطلبات الحصول على درجة الماجستير في العلوم الصيدلانية

قسم العلوم الصيدلانية

كليـة الصيدلـة

جامعة الشرق الأوسط

كانون الثاني، 2026

Thesis Committee Decision

This thesis, titled **"Evaluation of the Inhibitory Effects of Polyphenols from Elettaria Cardamomum Extract on Staphylococcus aureus, Collagenase, and Tyrosinase: In Vitro Investigations"** by researcher **AlAmeen Ahmed Hussien Alshaibany** and was successfully defended and approved on 25/01/2026.

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Last but not the least, I pray that this work may be sincere for the sake of the Almighty, and that it may serve as a stepping stone towards scholarly service that benefits society and contributes to the progress of my country, Iraq, and my second country, dear Jordan.

AlAmeen Alshaibany

Dedication

Thanks to my family for your lifelong love and support

I am grateful that you continued to have faith in me even when things were challenging

Dedicated to my friends, who have never failed to be there for me and cheer me on

You have made this lengthy journey simpler and more meaningful

To all of you, this accomplishment is dedicated

AlAmeen Alshaibany

Table of Contents

List of Tables

List of Figures

List of Appendices

List of Abbreviation

Abbreviation	Definition
ANOVA	Analysis of Variance
DMSO	Dimethyl Sulfoxide
DPPH	2,2-Diphenyl-1-picrylhydrazyl
E. cardamomum	Elettaria cardamomum
ECM	Extracellular Matrix
GAE	Gallic Acid Equivalent
GC-MS	Gas Chromatography–Mass Spectrometry
LC-MS/MS	Liquid Chromatography–Tandem Mass Spectrometry
MBC	Minimum Bactericidal Concentration
MIC	Minimum Inhibitory Concentration
MMPs	Matrix Metalloproteinases
PDB	Protein Data Bank
QE	Quercetin Equivalent
ROS	Reactive Oxygen Species
S. aureus	Staphylococcus aureus
SPSS	Statistical Package for the Social Sciences
TEAC	Trolox Equivalent Antioxidant Capacity
TFC	Total Flavonoid Content
TPC	Total Phenolic Content
UV	Ultraviolet

Evaluation of the Inhibitory Effects of Polyphenols from Elettaria Cardamomum Extract on Staphylococcus aureus, Collagenase, and Tyrosinase: In Vitro Investigations

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Abstract

Background: *Elettaria cardamomum*, is a plant species that contain natural substances polyphenols, that are well known to have strong antibacterial, enzyme-inhibitory, and antioxidant properties.

Aim: The aims of this study are to analyze the polyphenolic content of *E. cardamomum* ethanolic extract, and to evaluate the extract inhibitory effects on *Staphylococcus aureus* growth, antioxidant, Collagenase and Tyrosinase enzymes activities.

Methods: Ethanolic extract of *E. cardamomum* seeds were prepared, and the phytochemical constituents were identified using Folin-Ciocalteu, $AlCl_3$, LC-MS and GC-MS analysis. Antioxidant activity was determined using DDPH assay. Inhibitory effects on Collagenase and Tyrosinase enzymes activities were determined using in silico molecular docking tests.

Result: The content of total phenol and flavonoid compounds of extract of *E. cardamomum* extract were determined (1.78 mg equivalent GAE and 0.3 mg equivalent quercetin / g dry plant extract), respectively with maximum antioxidant activity observed at (0.04 mg/ mL). The LC/MS-MS analysis revealed that p-coumaric acid was the most abundant (3.08 µg/ ml), followed by caffeic acid, ferulic Acid, and rutin. GC-MS analysis identified α-Terpinyl acetate as a major characteristic aromatic constituent (11.15%), in addition to other terpenoid esters, fatty acids, and oxygenated volatile-derived compounds. The antimicrobial activity examined on *S. aureus* result on MIC and MBC concentration of (0.049 mg/g). Molecular docking of caffeic acid, ferulic acid, p-coumaric acid, and rutin against human tyrosinase and collagenase in silico tests, yielded stable binding poses confined within the catalytic pockets. Molecular docking results showed that caffeic acid and rutin as promising scaffolds for tyrosinase and collagenase inhibition, respectively.

Conclusion: This study revealed that ethanolic extract of *E. cardamomum* is rich with varied phenolic components with many biological activities. These findings are of special interest for researchers and consumers interested in natural products in the cosmetic and pharmaceutical fields. Therefore, further research is recommended before the real application of these findings can be further considered, if future development of novel naturally derived pharmaceutical formulations is considered.

Keywords: Antioxidants, Cardamomum Extract, Collagenase, Flavonoid, Polyphenolic, Staphylococcus Aureus, Tyrosinase.

تقييم التأثيرات المثبطة للبوليفينولات من مستخلص الهيل على المكورات العنقودية الذهبية والكولاجيناز والتيروزيناز: دراسات مخبرية

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إشراف

أ.د. ريم عدنان عيسى

الملخص

الخلفية: يُعد "الهيل" من الأنواع النباتية التي تحتوي على مواد طبيعية تُعرف بـ "البوليفينولات" (متعددات الفينول)، والتي تمتاز بخصائصها القوية المضادة للبكتيريا، والمثبطة للإنزيمات، والمضادة للأكسدة.

الهدف: تهدف هذه الدراسة إلى تحليل المحتوى الفينولي للمستخلص الإيثانولي لبذور الهيل، وتقييم آثاره المثبطة على نمو بكتيريا "المكورات العنقودية الذهبية"، ونشاطه المضاد للأكسدة، بالإضافة إلى تقييم قدرته على تثبيط نشاط إنزيمي "الكولاجيناز" و"التايروزيناز."

المنهجية: تم تحضير مستخلص إيثانولي من بذور الهيل، وتحديد المكونات الكيميائية النباتية باستخدام كاشف "فولين–سيوكالتو"، وكلوريد الألومنيوم، وتقنيات "الكروماتوغرافيا السائلة المقترنة بمطياف الكتلة " و"الكروماتوغرافيا الغازية المقترنة بمطياف الكتلة ."كما تم تحديد النشاط المضاد للأكسدة باستخدام اختبار "دي–بي–بي–إتش ."وتم تقييم التأثيرات المثبطة لنشاط إنزيمي "الكولاجيناز" و"التايروزيناز" عبر اختبارات "الإرساء الجزيئي المحوسب."

النتائج: أظهرت النتائج أن محتوى الفينولات الكلية والمركبات الفلافونيدية في المستخلص بلغت (1.78 مجم مكافئ لحمض الجاليك و0.3 مجم مكافئ للكويرسيتين لكل جرام من المستخلص الجاف) على التوالي، مع تسجيل أعلى نشاط مضاد للأكسدة عند تركيز (0.04 مجم/مل). وكشف تحليل الكروماتوغرافيا السائلة أن "حمض البي–كوماريك" كان الأكثر وفرة (3.08 ميكروجرام/مل)، يليه حمض "الكافيك"، وحمض "الفيروليك"، ومركب "الروتين". كما حدد التحليل الغازي مركب "ألفا–تيربينيل أسيتات" كمكون عطري رئيسي (11.15%)، بالإضافة إلى استرات التربينويد، والأحماض الدهنية، والمركبات المتطايرة المؤكسجة. وبالنسبة للنشاط المضاد للميكروبات، بلغت قيم "التركيز المثبط الأدنى" و"التركيز القاتل الأدنى" ضد بكتيريا المكورات العنقودية الذهبية (0.049 مجم/جم). وأسفرت نتائج الإرساء الجزيئي لكل من حمض الكافيك، والفيروليك، والبي–كوماريك، والروتين ضد إنزيمي التايروزيناز والكولاجيناز البشري عن روابط مستقرة داخل الجيوب التحفيزية للإنزيمات. وأثبتت النتائج أن حمض الكافيك والروتين يمثلان ركائز واعدة لتثبيط التايروزيناز والكولاجيناز على التوالي.

الاستنتاج: خلصت الدراسة إلى أن المستخلص الإيثانولي للهيل غني بمكونات فينولية متنوعة تمتلك أنشطة بيولوجية متعددة. وتعد هذه النتائج ذات أهمية خاصة للباحثين والمستهلكين المهتمين بالمنتجات الطبيعية في مجالات التجميل والصيدلة. لذا، يوصى بإجراء مزيد من الأبحاث قبل التطبيق الفعلي لهذه النتائج في تطوير تركيبات صيدلانية مبتكرة مشتقة من مصادر طبيعية.

الكلمات المفتاحية: مستخلص الهيل، البوليفينولات، الفلافونيدات، مضادات الأكسدة، المكورات العنقودية الذهبية، التايروزيناز، الكولاجيناز

Chapter One
Background and Problem Statement

1.1 Staphylococcus aureus, Collagenase, and Tyrosinase

Staphylococcus aureus is a gram-positive bacterium that causes serious sickness and death worldwide. It is a major contributor to infections of the skin and soft tissues, particularly *Acne vulgaris*, which is a chronic inflammatory skin condition (Kirsten et al., 2021; W.Levinson&E.Jawetz, 2000). Acne can also be caused by hormonal abnormalities (Elsaie, 2016). In addition, infections of the skin and soft tissues are also frequently being caused by Methicillin-resistant *S. aureus* (MRSA) (Donkor et al., 2019; Hassoun.et.al, 2017). One of the current challenges is the pressing need for innovative treatments from non-traditional sources such as plant seeds, plant roots and herps (Maddiboyina et al., 2023).

Collagenases are proteinases that are part of the family of zinc-dependent endopeptidases known as matrix metalloproteinases (MMPs). MMP-1, MMP-8, and MMP-13 are collagenases that break down collagen to remodel the extracellular matrix (ECM) (Madzharova et al., 2019). The most prevalent structural protein found in the extracellular matrix (ECM) that preserves tissue integrity is collagen type I (Kisling et al., 2019). Numerous human disorders, including cancer, heart disease, neurological diseases, and arthritis, can be linked to uncontrolled collagen degradation.

As the skin ages, one of the primary reasons for wrinkles and a lack of firmness is the depletion of collagen (Ågren et al., 2020; Amar et al., 2017). Reactive oxygen species (ROS) can indirectly trigger the formation of MMPs through the MAP-kinase pathway when exposed to ultraviolet (UV) light (Gu et al., 2020). Therefore, the pharmaceutical and cosmetic industries have made collagenase a key target (Avila Rodríguez, 2018). On the other hand, an enzyme called tyrosinase, which contains copper, hydroxylates L-tyrosine to 3,4-dihydroxyphenylalanine (L-DOPA), which is then converted by the melanin pathway to L-dopaquinone. In order for the skin to produce pigments, this enzyme is necessary (Olsson and Gillbro, 2011). Natural defenses against sun radiation damage are provided by these pigments (Bae-Harboe and Park, 2012).

The overproduction of melanin is linked to hyperpigmentation issues such as melasma, freckles, solar lentigo (Age Spots), and post-inflammatory hyperpigmentation,

despite the pigment's vital physiological roles (Speeckaert et al., 2014). Both internal and environmental variables, including UV exposure, are linked to the increased production of melanin. Tyrosinase inhibition is a desirable target for pigmentation disorders or cosmetic applications because it can stop the buildup of melanin in the skin (Gu et al., 2020). Herbal remedies have recently gained popularity in cosmetics as a way to treat skin problems (Apraj, 2016). By reducing the activity of collagenase and tyrosinase, herbal-derived active compounds have the potential to have beneficial effects. One example of this is the delay in the degradation of collagen and other components of the extracellular matrix (Al-Halaseh et al., 2022).

1.2 The nature of the compounds: Polyphenols

Polyphenols, plant secondary metabolites, are vital to plant systems. They shield against parasites, insects, UV radiation, and other environmental hazards (Troncozo et al., 2019). Additionally, polyphenols are antioxidants, anti-inflammatory, anti-mutagenic, anti-cancer, and anti-proliferative (Ciupei et al., 2024). Flavonoids, phenolic acids, tannins, and stilbenes are the four categories that are used to categorise polyphenols. Because of its great antioxidant potential, it has been the subject of a significant amount of research into its capability to neutralize free radicals, protect cellular structures, and modify biological pathways that are involved in inflammation, ageing, microbial infection, and carcinogenesis (Scalbert et al., 2005).

Polyphenols' antioxidant, anti-inflammatory, antibacterial, anti-collagenase, and anti-tyrosinase qualities make them useful in pharmaceutical and cosmeceutical industries. Polyphenols are beneficial in topical formulations for skin infections, hyperpigmentation, and premature ageing (Ciupei et al., 2024).

1.3 Elettaria Cardamomum

The *Elettaria cardamomum* plant, which is mostly cultivated in South India and Sri Lanka, is a spice that is both pricey and old (Lwasa, 2007). Arabs use its seeds as a spice, medicinal, and to flavor pastries, coffee, and curries. A small amount is employed in pharmacies as compound tinctures and in liqueurs. In addition, cardamom seeds produce 4% volatile oils, mostly terpinyl acetate and cincole with trace amounts of alcohols and esters (Lewis, 2025).This species has been used in Ayurvedic and Unani medicine for ages to heal respiratory and digestive disorders. Recent studies have revealed that it is

antibacterial, anti-inflammatory, and may prevent chemotherapy (Suhail et al., 2010). According to Anand et al. (2007), E. cardamomum seeds contain phenolic acids like caffeic and ferulic acid, flavonoids like quercetin, and essential oils like 1,8-cineole and α-terpinyl acetate, indicating their potential as a medicinal agent.

Most study on essential oils from E. cardamomum has not focused on polyphenolic content or enzyme inhibition. To our knowledge, few studies have examined cardamom polyphenols' ability to inhibit S. aureus, collagenase, and tyrosinase. Due to this research void, cardamom polyphenol extracts' multi-target potential for pharmacological and cosmetic formulations and uses may be explored.

1.4 Aims of the study

The main aims of this study is to evaluate the polyphenolic content and the inhibitory effects of *E. cardamomum* ethanolic extract on *S. aureus* bacterial growth, free radical scavenging, and activity of tyrosinase and collagenase enzymes. In doing so, it might be the foundation for the development of new natural bioactive ingredients, that are suitable for topical drug delivery systems, especially for use in antimicrobial skincare, anti-aging treatments, and anti-pigmentation effects.

1.5 Study Questions

1. What is the total content of phenols and flavonoids in the ethanolic extract of *E. cardamomum?*
2. What is the phenolic profile in the ethanolic extract of *E. cardamomum* obtained using LC-MS/MS analysis*?*
3. What is the terpenoids profile in the ethanolic extract of *E. cardamomum* obtained using GC-MS analysis*?*
4. What is the minimum inhibitory concentration (MIC) of the ethanolic *E. cardamomum* extract against *S. aureus*?
5. Is there an antioxidant effect of ethanolic extract of *E. cardamomum* on free radical reactions?
6. Is there an inhibition effect of ethanolic extract of *E. cardamomum* on collagenase enzymes activity?
7. Is there an inhibition effect of ethanolic extract of *E. cardamomum* on tyrosinase enzymes activity?

1.6 Study Objectives:

1. To perform phytochemical and antioxidant screening tests of *E. cardamomum* ethanolic extract using standard procedures.
2. To analysis the phenolic and terpenes profiles *E. cardamomum* ethanolic extract using LC-MS/MS and GC-MS methods.
3. To evaluate *E. cardamomum* ethanolic extract antibacterial efficacy against *S. aureus*.
4. To determine the MIC against *S. aureus* for *E. cardamomum* ethanolic extract.
5. To assess the inhibition effects of the *E. cardamomum* ethanolic extract on collagenase and tyrosinase enzymes activity.

1.7 Study Significance:

This research is expected to make significant improvements to the scientific and pharmaceutical in natural products research area, by addressing a gap in the body of knowledge regarding *Elettaria cardamomum's* polyphenolic chemicals and their activities. As the essential oil extract of cardamom has been the focus of many previous researchers, nevertheless, its polyphenolic components and their inhibitory effects against microbial pathogens and important skin-related enzymes have received limited attention in the literature.

1.8 Beneficiaries:

The following important stakeholders are expected to benefit by this study:

- **The findings may assist the pharmaceutical and cosmetic industries:** develop natural antimicrobial, anti-aging, and skin-lightening products with cardamom polyphenols as active ingredients.
- **Academic and Research Institutions:** Future pharmacogenetic, microbiological, and biochemical research can be built upon the new understanding of the pharmacological uses of *Elettaria cardamomum* polyphenols that the study will offer.
- **Healthcare Professionals:** By developing an improved understanding of plant-based alternatives for synthetic antimicrobial and enzymatic agents, dermatologists and chemists may be more knowledgeable to recommend safer and more environmentally friendly treatment options.

- **Natural therapists and product formulators:** The information could help formulators that use plant-based and herbal ingredients optimize therapeutic skincare and health supplements.
- **Patients and Customers:** New researched natural formulations could benefit the public searching for natural treatments for bacterial skin infections, hyperpigmentation, and early skin ageing.

1.9 Contribution to Scientific Knowledge

This study focusses on a major gap in the current literature, which benefits the scientific community:

- It develops our knowledge of the phytochemical and bioactivity profile of *E. cardamomum* performing researched focuses on the polyphenolic fraction.
- The multi-target inhibitory effects of cardamom polyphenols on *S. aureus*, collagenase, and tyrosinase—three therapeutically and cosmetically significant targets—are presented for the first time in this study.
- It provides a more comprehensive approach to treating skin-related disorders by introducing the potential of multifunctional plant extracts for use in topical pharmaceutical and cosmeceutical products.

Therefore, this research is expected to enhance the scientific basis for the development of sustainable natural products in the fields of dermatology, cosmetic science, enzymology, and microbiology.

1.10 Organization of Thesis:

This thesis has five main chapters, each arranged logically and methodically to provide coherence between theoretical background, experimental techniques, results, and scientific interpretation. These chapters are organized as follows:

Chapter one introduction: This chapter discusses the study's science. Introductions to Staphylococcus aureus, collagenase, tyrosinase, and natural polyphenolic compounds are discussed. This article emphasizes Elettaria cardamomum. The chapter also covers the research topic, aims, questions, objectives, relevance, beneficiaries, and scientific contribution.

Chapter Two Literature review: This chapter discusses Elettaria cardamomum's phytochemical composition, medicinal and pharmacological properties, and biological activities of its phenolic and terpenoid constituents, as well as important prior studies and scientific literature. Discussing antimicrobial activity and enzyme inhibition (collagenase and tyrosinase) studies illustrates the research gap that the present study filled.

Chapter Three Materials and Method: This chapter describes the research instruments, chemicals, and materials. It describes the preparation of the ethanolic extract of E. cardamomum seeds, phytochemical screening, LC-MS/MS analysis of phenolic compounds, GC-MS analysis of terpenoid compounds, antioxidant and antimicrobial assays, in silico enzyme inhibition studies, and statistical analysis.

Chapter Four Result: This chapter presents the study's experimental and analytical results. These discoveries include extraction yield, phytochemical screening, antioxidant activity, phenolic and terpenoid component chromatographic identification, antibacterial activity, and collagenase and tyrosinase inhibition molecular docking.

Chapter Five Discussion and conclusion: This chapter summarizes the key findings, compares them to earlier research, analyses the biological significance of the chemicals found, explains the study's limitations, and describes the compounds found. It also suggests medicinal and cosmetic uses and additional research.

Chapter Two
Theoretical Framework and Previous Studies

2.1 Introduction

Nowadays, the impacted of the phenomena of bacterial resistance, is recognized with many of antibiotic families. Both quantitative and qualitative resistance are present. The WHO reports that over 80% of the world's population uses medicinal plants to treat various diseases (Cisneros-Zevallos, 2021).

This has generated a great deal of interest, in developing novel medications or preparations, from natural sources such as plants derived drugs. In traditional medicine, plant extracts and plant-derived substances serve as a natural model for the creation of novel pharmaceuticals, and serve as the foundation for drug development (Moulai-Hacene et al., 2020). In addition, numerous Ayurvedic plants show promise as broad-spectrum antimicrobials. Alkaloids, anthraquinones, cardiac glycosides, saponins, tannins, and polyphenols are the primary antimicrobial phytocompounds (Alkhalifah et al., 2022). The natural plant substances called polyphenols have strong antibacterial, enzyme-inhibitory, and antioxidant properties (Scalbert et al., 2005). Numerous therapeutic plants contain them, and they act by scavenging free radicals, preventing the growth of bacteria, and blocking enzymes that are involved in inflammation and pigmentation reactions (Daglia, 2012).

Flavonoids like quercetin and catechins inhibited S. aureus, including MRSA, in multiple trials (Cushnie and Lamb, 2011). These polyphenols tear down bacterial membranes, block enzymes, and enhance antibiotic efficacy. Herbal medicines from the genus: Elettaria cardamomum, the "queen of spices" herbaceous perennial, is in Zingiberaceae. The seed has phenols, tannins, starch, terpinoids, proteins, avonoids, and sterols (Kawatra et al., 2023).

Green cardamom, or *E. cardamomum*, is a species that is frequently used in traditional medicine to treat respiratory and digestive conditions. Antibacterial, antifungal, and antioxidant qualities have been demonstrated by its essential oil (Suhail et al., 2010; Al-Zuhair et al., 2018). A matrix metalloproteinase called collagenase enzyme breaks down collagen, which causes tissue damage and ageing of the skin. It has been shown

that polyphenols like ferulic acid inhibit collagenase, which turns them appeal for anti-aging treatments (Brinckerhoff and Matrisian, 2002).

Hyperpigmentation results from the overactivity of tyrosinase, an enzyme essential for the synthesis of melanin. Synthetic inhibitors like hydroquinone can have negative effects. Therefore, safer alternatives are provided by natural inhibitors; including flavonoids and gallic acid (Parvez et al., 2006; Chang, 2009).

The combination of inhibitory effects of *E. cardamomum* polyphenols on *S. aureus*, collagenase, and tyrosinase enzymes have not been assessed in any previously published research, despite the promising activities of plant-derived polyphenols. This establishes a gap in literature, supporting the current research hypothesis.

2.2 Origin of Elettaria cardamomum

In its natural state, Elettaria cardamomum, Maton is a plant that is indigenous to the nation of India. Despite this, cultivation of this spice can also be found in the countries of Guatemala, Ski Lanka, Nepal, Vietnam, Laos, and El Salvador. This is because market demand and commercial interest are driving the cultivation of this spice. *O*ver 85% of the world's cardamom (*Amomum subulatum*) is grown in India, with the biggest yearly output of 4000 metric tons being produced in Nepal (2500 metric tons) and Bhutan (1000metric tones) (Pathak et al., 2025).

2.3 Types of Cardamom

Cardamom comes in two primary varieties: little (green) and large (black) (Figure 2.1). The most commonly grown type of cardamom is green cardamom, which has a small biological source (*E. Cardamomum*), whereas black cardamom is primarily grown in India. Table 2. 1 shows a comparison of the organoleptic properties between the two types of cardamomum species (Azgomi et al., 2024).

Figure 2.1: Types of Cardamom (Azgomi et al., 2024).

Table 2.1: A comparison of the organoleptic properties between the two types of cardamomum species.

Parameter	Green cardamom	Black cardamom
Scent and flavor	It has a strong scent and flavor.	It has a scent and flavor that is slightly camphor-like and smokey.
Plant species	Elettaria cardamomum is the plant species that produces the spice called green cardamom.	Amomum subulatum is the plant species that produces the spice called black cardamom.
Part of plant	Pods and seeds are both used.	Only seeds are being used

Table 2.1 compares the organoleptic and botanical qualities of green and black cardamom. Green cardamom, from Elettaria cardamomum, is valued in culinary, medicinal, and pharmaceutical applications for its strong, pleasant aroma and intense flavor. The scent of black cardamom, from Amomum subulatum, is more camphor-like and smoky. Both the pods and seeds of green cardamom are used botanically and practically, while black cardamom is only used as seeds. The two cardamom species differ in sensory attributes, plant origin, and utilization patterns, which may affect their chemical composition, biological activities, and suitability for therapeutic and industrial uses.

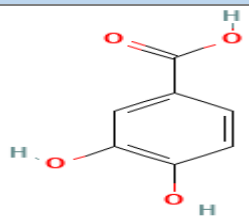
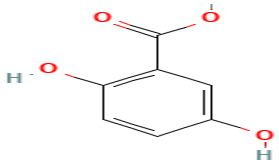
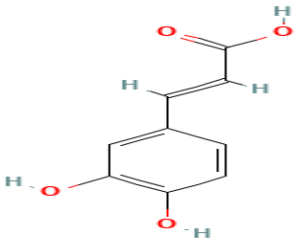
2.4 Phyto chemical composition of cardamomum

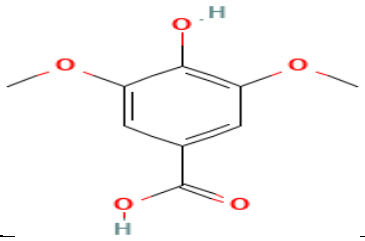
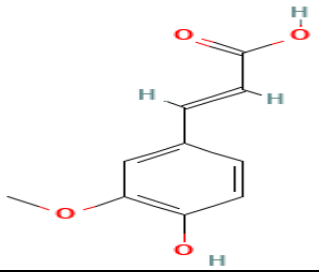
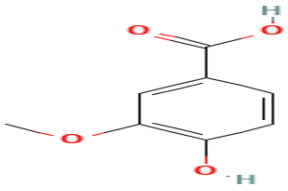
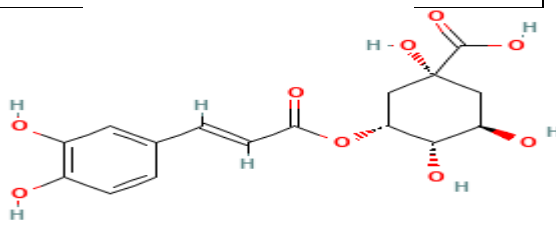
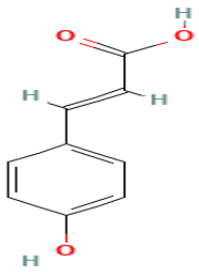
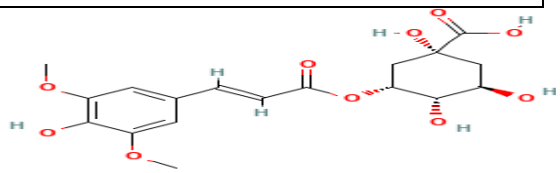
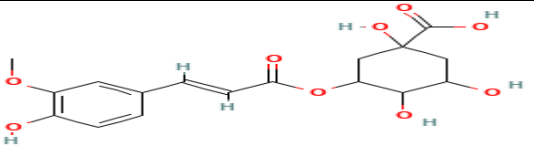
2.4.1 Phenolic component of cardamomum

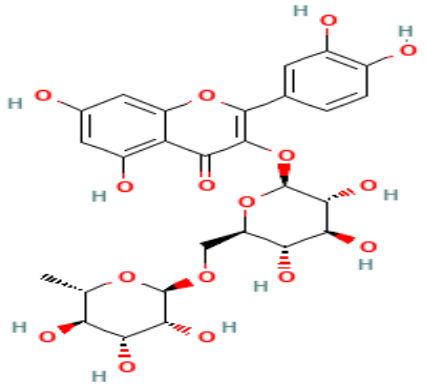
Phenols are aromatic compounds that have one or more hydroxyl groups integrated into their structure. It is possible for phenols to contain other substitutes, particularly methyl groups, in addition to the aromatic benzene ring system. When it comes to phenols, the most basic structures are C6 structures, which consist of an aromatic ring that is attached to a hydroxyl group. The phenols distribution of these organisms is widespread across all categories of plant life. The bactericidal, antiseptic, and anthelmintic properties of simple phenols are the general properties of these compounds (Al-Maliki, 2011).

Whole cardamom is rich in phenol and terpenoid compounds, with ~141.5 mg phenolics/100 g and 416 mg essential oil/100 g. Table (2.2) shows LC-MS/MS determined cardamom, skin, and seed phenolic content. However, cardamom phenolics have anti-inflammatory and other effects (Sreedharan et al., 2023).

Table 2.2: Phenolic content in cardamom, skin, and seed detected by LC-MS/MS (Sreedharan et al., 2023).

Phenolic compound	Content (%) (mg/100 g)	Molecular Formula	Structure
Protocatechuic acid	23.48	$C_7H_6O_4$	
Gentisic acid	1.14	$C_7H_6O_4$	
Caffeic acid	29.51	$C_9H_8O_4$	

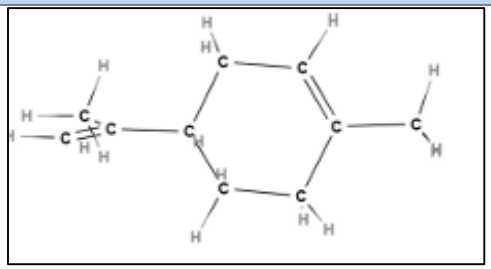
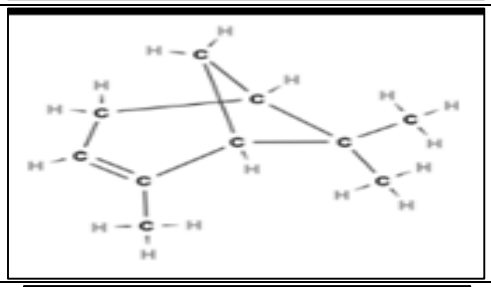
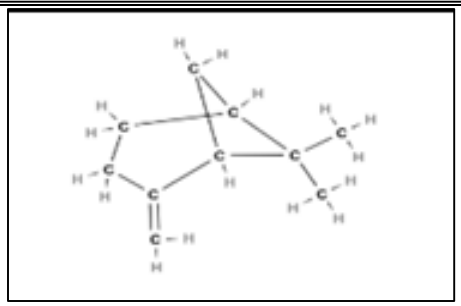
Phenolic compound	Content (%) (mg/100 g)	Molecular Formula	Structure
Syringic acid	34.11	$C_9H_{10}O_5$	
Ferulic acid	8.51	$C_{10}H_{10}O_4$	
Vanillic acid	4.99	$C_8H_8O_4$	
5-O-caffeoylquinic acid	28.96	$C_{16}H_{18}O_9$	
p-coumaric acid	3.53	$C_9H_8O_3$	
Sinapoyl quinic acid	5.79	$C_{18}H_{22}O_{10}$	
Feruloyl quinic acid	0.97	$C_{17}H_{20}O_9$	

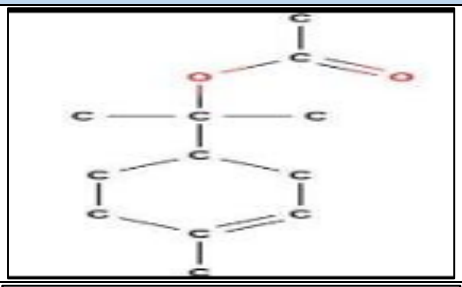
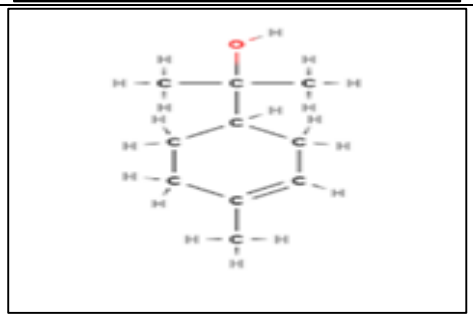
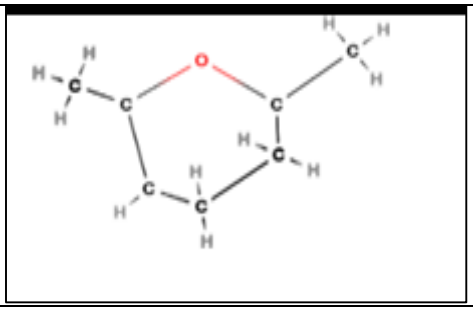
Phenolic compound	Content (%) (mg/100 g)	Molecular Formula	Structure
Rutin	0.57	$C_{27}H_{30}O_{16}$	

2.4.2 Terpenes compounds of cardamom

According to Taherzadeh et al. (2025), cardamom contains a variety of terpenoid chemicals, including limonene, α, β- pinene, α- terpinyl acetate, α -terpineol and 1,8-cineole. These compounds are listed in Table (2.3).

Table 2.3: Terpenoid compounds present in cardamom.

Terpens	Chemical formula	Properties	Chemical structure
Limonene	($C_{10}H_{16}$).	Its molecular weight is (136.23). Its IUPAC name is (1-methyl-4 prop- 1-en-2 ylcyclohexene).	
α-pinene	($C_{10}H_{16}$).	Its chemical formula is α-pinene also known as Acintene A, alpha.-Pinene. Its molecular weight is (136.23).	
β-pinene:	($C_{10}H_{16}$)	It is β-pinene is also known as 2(10)-Pinene. Its molecular weight is (136.23). It is colorless and transparent liquid.	

Terpens	Chemical formula	Properties	Chemical structure
α-terpinyl Acetate	($C_{12}H_{20}O_2$).	Its IUPAC name is (2-(4 methylcyclohex-3-en-1-yl) propan-2- yl acetate).	
α-terpineol	($C_{10}H_{18}O$)	It is also known as (2-4- methylcyclohex-3-en-1-yl). Its Molecular weight is (154.25).	
1,8-cineole	($C_{10}H_{18}O$)	It is also known as Eucalyptol. Its molecular weight is (154.25).	

2.5 Therapeutic Uses of *E. Cardamomum*

E. cardamomum, has a varied phytochemical profile, all of which contribute to its well-known medicinal benefits. These bioactive components have led to its extensive use in traditional medical systems like Chinese, Ayurvedic, and Unani medicine (Banerjee et al, 2024). Several pairs of conditions and diseases, including asthma, tooth infections, digestive and kidney disorders, diarrhea, nausea, cataracts, and cardiac disorders, are among the most common conditions that are treated with this medication. In addition, cardamom capsules are frequently utilized as flavoring agents in the cuisine of Middle Eastern and Indian cuisine types. It possesses several pharmacological traits, such as antioxidant, anti-cancer, anti-inflammatory, anti-microbial, cardio-protective, diuretic, gastro-protective, immunomodulatory, and sedative, with tremendous food and medical applications (Cheikhyoussef et al., 2023).

Recent research has shown that cardamom extract modulates macrophages and protects against uranium risks. The antibacterial and antifungal qualities of cardamom

extract are widely known. This plant has been shown to have analgesic, depressive, anticonvulsive, and antispasmodic properties (Mohammed et al., 2024). In addition, it is effective in treating infections of the gums, teeth, and throat, as well as lung congestion, tuberculosis, excessive blood pressure, heart disease, and digestive issues. According to Yahyazadeh et al. (2021), the anticancer benefits of cardamom are derived from its anti-inflammatory, anti-proliferative, pro-apoptotic, and antioxidant qualities.

2.6 Roles of Cardamom as an Essence of Life

E. Cardamomum represents health, vigor, and harmony, and is an essential part of human existence due to its rich phytochemical qualities, cultural importance, and medicinal effects. Its use in religion, traditional medicine, and international cuisine shows its importance to human health. Cardamom adds richness and energy to life as a spice, medicine, or symbol (Kumar and Kumari, 2021).

2.7 Pharmacological Activity of *E. Cardamomum*

2.7.1 Cardamom as a Spice

Black cardamom is more powerful and smokier than green cardamom, which is regarded to be pleasant and aromatic. Green cardamom is often used in culinary applications. Several Indian desserts, like kheer and gulab jamun, include it as an ingredient in their preparation. According to the findings of study conducted by Kawartra et al. (2023), it also enhances the flavour of traditional Scandinavian meals such as cardamom buns. There are also desserts like cakes, puddings, and custards that can reap the benefits of the enhancing process.

2.7.2 Cardamom Tea

Cardamom tea is both delicious and beneficial to one's health because it contains vitamins, essential oils, and antioxidants. In addition, gas, bloating and indigestion may benefit from cardamom tea. Additionally, it promotes the production of digestive enzymes, which enhances digestion and may reduce heartburn and acid reflux symptoms. It also supports renal function, helps the body eliminate toxins, and, because of its diuretic properties, may help prevent urinary tract infections (Kawatra et al., 2023).

2.7.3 Antiseptic

There are essential oils that may be discovered in cardamom, including borneol, limonene, α-terpineol, and 1,8-cineole (eucalyptol). These oils have the ability to influence the membranes of microbial cells, so preventing the growth of bacteria. Using cardamom can prevent bacteria, mould, and viruses successfully. Also, E. Cardamom kills bacteria, heals, and reduces inflammation, making it a natural antiseptic. However, with more research and clinical testing, its pharmacological and medical uses may rise (Souza et al., 2024).

2.7.4 Anti-inflammatory

The presence of a wide variety of phytochemicals, including 1,8-cineole (eucalyptol), limonene, terpinene, borneol, and flavonoids, which are all abundant in cardamom, makes *E. Cardamomum* a good treatment for the treatment of disorders that are caused by inflammation. It is the presence of these substances that inhibits the synthesis of cytokines and other mediators that promote inflammation. Furthermore, cardamom has powerful antioxidant properties, which makes it an indirect anti-inflammatory agent. It does this by lowering the amount of free radicals in the body. Additionally, cardamom has the ability to decrease the formation of inflammatory mediators including prostaglandins and leukotrienes by inhibiting enzymes such as cyclooxygenase and lipoxygenase (Kumar et al., 2022).

2.7.5 Antimicrobial

E. Cardamomum is efficient against a variety of bacteria, fungi, and viruses due to its strong antibacterial properties. These properties are mostly attributed to the presence of a multitude of bioactive phytochemicals and essential oils, which include borneol, limonene, α-terpineol, and 1,8 cineole, as stated by Patel et al (2024). With inhibition zone diameter (IZD) values ranging from (11.9 to 26.8 mm) and minimum inhibitory concentration (MIC) values of (0.25 and 0.50 mg/disc) against S. aureus, the extract demonstrated the highest antibacterial activity against the tested strains, according to the findings of an in vitro study on the antimicrobial potency of E. cardamomum extract against S. aureus (ATCC 29213) (Yassin et al., 2022). An aqueous extract of green cardamom, rich in flavonoids with reducing properties, was used to test plant antibacterial activities against Gram-positive (S. aureus and B. subtilis) bacteria (Pal et al., 2020).

Cardamom extract into sodium alginate (SA): polyvinyl alcohol (PVA) mat to design a wound dressing scaffold by electrospinning method and reported its antibacterial activities against *E. coli* and *S. aureus,* with a significant reduction in the bacterial growth of (97% and 99%), respectively (Najafi et al.,2021). Nearly every tested microbial strain is inhibited by the ethanolic extract of Elettaria cardamomum (EEC). Different microbial species and EEC concentrations have varying degrees of this effect. The findings demonstrate the range of action of cardamom against both Gram-positive and Gram-negative bacteria. Also, EEC exhibits antifungal activity against yeast at all concentrations, while at low concentrations, EEC partially inhibited mould (Moulai-Hacene et al., 2020).

2.7.9 Anti-cancer

Preclinical research on *E. Cardamomum* has shown positive anti- cancer characteristics, as it is abundant in flavonoids and phenolic compounds which reduce oxidative stress, a major factor in the development of cancer, and also neutralize free radicals. Furthermore, its extracts provide cancer cells apoptosis, or programmed cell death, by activating pathways like the mitochondrial (intrinsic) apoptotic pathway, in addition to modulating important signaling pathways such as nuclear factor kappa B (NF-κB), mitogen-activated protein kinase (MAPK), and PI3K/Akt, which are frequently dysregulated in cancer (Patel et al., 2024). Chronic inflammation increases cancer risk, while cardamom inhibits angiogenesis, the process of creating new blood vessels for tumour growth and dissemination. Anti-inflammatory plant extract may reduce cancer risk by suppressing pro-inflammatory cytokines. Although preclinical research is promising, further human clinical trials are needed to determine its safety and efficacy in cancer prevention and therapy (Mohammed et al., 2024).

2.8 Summary of literature review

The literature shows that medicinal plants are becoming more popular as sources of bioactive compounds that can treat microbial resistance, oxidative stress, and enzyme-related skin disorders. Many studies have shown that plant-derived polyphenols have antioxidant, antimicrobial, anti-inflammatory, and enzyme inhibitory properties, making them promising pharmaceutical and cosmeceutical candidates.

Polyphenolic compounds like phenolic acids and flavonoids have been shown to have strong antioxidant activity through free radical scavenging, metal chelation, and oxidative

stress pathway modulation. These properties safeguard cellular structures and slow ROS-induced skin ageing. Polyphenols disrupt bacterial cell membranes, inhibit essential enzymes, and disrupt microbial metabolic pathways, killing Gram-positive bacteria like Staphylococcus aureus, according to several studies.

The literature emphasises collagenase and tyrosinase enzymes' clinical and cosmetic value. Collagenase, a matrix metalloproteinase, degrades collagen, causing skin elasticity loss and wrinkles. However, hyperpigmentation disorders are linked to tyrosinase overactivity, a melanin biosynthesis enzyme. Numerous studies show that natural phenolic compounds can inhibit these enzymes, offering safer alternatives to synthetic inhibitors with side effects.

The reviewed studies confirm Elettaria cardamomum's long history in traditional medicine and rich phytochemical composition. Essential oils, terpenoids, phenolic acids, flavonoids, and other secondary metabolites with various pharmacological effects have been found in the plant. Most research on E. cardamomum essential oil has focused on its antioxidant, antimicrobial, anti-inflammatory, and anticancer properties. Commonly, α-terpinyl acetate and 1,8-cineole are identified as key constituents causing these effects.

The literature shows a limitation and research gap in E. cardamomum polyphenolic fraction. Some studies have identified individual phenolic compounds, but few have combined phenolic profiling with biological antimicrobial activity and enzyme inhibition. Few studies have used an integrated experimental and computational approach to test E. cardamomum polyphenols' inhibitory potential against Staphylococcus aureus, collagenase, and tyrosinase.

Although molecular docking and in silico studies are increasingly used to predict enzyme–ligand interactions for plant-derived compounds, they are rarely used for E. cardamomum polyphenols. This emphasises the need for phytochemical characterization and molecular mechanistic studies.

Plant-derived polyphenols and Elettaria cardamomum have therapeutic and cosmetic potential, according to the literature. However, it highlights a significant knowledge gap regarding E. cardamomum ethanolic extract polyphenolic composition and multi-target biological activities. This study fills this gap by assessing E. cardamomum polyphenols' phytochemical profile, antimicrobial efficacy, antioxidant activity, and enzyme inhibitory potential, adding new and integrated scientific evidence to the body of knowledge.

Chapter Three

Methodology (Methods and Procedures)

This chapter describes the materials, chemicals, instruments, and experimental procedures used to study Elettaria cardamomum seed ethanolic extract phytochemical composition and biological activities. The methods used in this study were carefully chosen to ensure reliability, reproducibility, and scientific validity and to meet Chapter One's research objectives. The chapter describes plant collection, extraction, and phytochemical screening to determine total phenolic and flavonoid content and antioxidant activity. LC-MS/MS and GC-MS were used to identify and quantify phenolic and terpenoid compounds, completing the extract's chemical characterization. The extract's antimicrobial activity against Staphylococcus aureus was assessed using microbiological assays to determine its minimum inhibitory and bactericidal concentrations. We used in silico molecular docking to study the interaction of selected phenolic compounds with collagenase and tyrosinase enzymes to determine their enzyme inhibitory potential. Finally, the statistical data analysis methods for accurate experimental interpretation. This systematic description of materials and methods creates a solid experimental framework that supports the findings in later chapters.

3.1 Equipments and Materials

The materials, reagents, and instruments that were utilised in the present investigation are detailed in Table (3.1), which can be found here.

Table 3.1: List of Materials and Equipment Used.

Item	Manufacturer / Source
Dried seeds of *Elettaria cardamomum*	AlRayhan, Amman, Jordan
Staphylococcus aureus	(ATCC 25923), a standard reference Gram-positive strain
Ethanol (99%)	Sigma-Aldrich or equivalent
Rotary evaporator	Heidolph or equivalent
UV–Vis Spectrophotometer (Model: U-1800)	Hitachi, UK
Analytical Balance	Mettler Toledo or equivalent
Centrifuge	Hettich Universal 320
Vortex Mixer	IKA or equivalent

Item	Manufacturer / Source
Freeze Dryer / Lyophilizer	Martin Christ or equivalent
Trolox (standard antioxidant)	Sigma-Aldrich
DPPH (radical reagent)	Sigma-Aldrich
Gallic Acid (standard phenolic)	Sigma-Aldrich
Quercetin (standard flavonoid)	Sigma-Aldrich
Aluminum chloride ($AlCl_3$)	Sigma-Aldrich
Sodium carbonate (Na_2CO_3)	Sigma-Aldrich
Formic acid (LC/MS grade)	Sigma-Aldrich
Methanol, Acetonitrile, Deionized Water (LC/MS)	Sigma-Aldrich
Dimethyl sulfoxide (DMSO, analytical grade)	Sigma-Aldrich

3.2 Plant Material

The plant *E. cardamomum* (L.) was purchased from a local herbal provider in Amman, Jordan. The pods were carefully removed, washed with sterile water to eliminate any contaminants, and then allowed to dry in the shade at room temperature until their weight remained constant. The dried pods were ground into a fine powder using a clean electric grinder.

3.2.1 Extraction

To extract the plant material, we mixed 200 g of powdered plant material with 1000 mL of pure ethanol. The mixture was allowed to macerate in a dark, room-temperature environment for a full day. Rotavapor was used to evaporate the ethanol and concentrate the recovered ethanolic extract following filtration with Whatman No. 1 paper catch particles larger than 10 μm. After performing additional lyophilization on the extract, it was finally dried and placed in a dark glass vial; it was then stored at 4 ° C until required.

3.3 Phytochemical Screening tests

3.3.1 Determination of Total Phenolic Content

The total phenolic content of *E. cardamomum* ethanolic leaf extract was determined using the Folin–Ciocalteu (FC) colorimetric assay, folin reagent is acidic (oxidants), following the procedure described by Sadeghi et al. (2015). The process of the test involves phenolic compound reduction of the FC reagent in a basic environment, which results in the creation of a blue chromophore that can be measured at 765 nm.

A stock solution of *E. cardamomum* ethanol extract was prepared at a concentration of 10 mg/mL in 1% ethanol. Serial dilutions were then prepared for analysis at serial concentrations of (0.25, 0.5, and 1.0 mg/mL). Gallic acid (GA) was used as the standard phenolic compound for constructing the calibration curve. A series of GA standards were prepared in the concentration range of (1–100 µg/mL).

For sample or standard solution, 1.0 mL of extract/ GA solution was pipetted into a 5.0 mL of distilled water and 1.0 mL of freshly prepared Folin–Ciocalteu reagent. The mixture was gently mixed and allowed to stand in the dark for 5 minutes. 1.0 mL of 7.5% sodium carbonate (Na_2CO_3) solution to neutralize the acid and raise the PH to the required level then added to initiate the color development. The tubes were covered with aluminum foil to protect from light and incubated at room temperature (~25°C) for 30–60 minutes.

The absorbance of each reaction mixture was measured at 765 nm using a UV–Vis spectrophotometer (Hitachi U-1800, UK). Total phenol content was calculated by substituting the absorbance values into the linear equation to obtain gallic acid equivalents. All measurements were measured in triplicates. The average and standard deviations were used for further calculations.

3.3.2 Determination of Total Flavonoid Content

Following the procedure outlined by Chang et al. (2002), a few small adjustments were made to the Aluminium chloride test in order to ascertain the total flavonoid content. An ethanol stock solution of *E. cardamomum* extract containing 0.01 g/ml was prepared. A mixture of 2.8 mL of distilled water, 1.5 mL of 95% ethanol, 0.1 mL of 10% Aluminium chloride, and 0.5 mL of the prepared solution was combined. The mixture was incubated at room temperature for 30 minutes before measuring its absorbance at 415 nm.

A stock solution of quercetin was prepared by dissolving 10 mg in 80% ethanol. Serial concentrations were prepared in the range of (25, 50, and 100 µg/mL) and used to prepare the calibration curve and used for the calculation of total flavonoid content in the extract expressed as equivalent to quercetin. All measurements were measured in triplicates. The average and standard deviations were used for further calculations.

3.3.3 Determination of Antioxidant Activity (Using DPPH assay)

The antioxidant capacity of *E. cardamomum* ethanolic extract was evaluated using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay and expressed as Trolox Equivalent Antioxidant Capacity (TEAC). The DPPH assay relies on the reduction of the stable violet-colored DPPH radical to a yellow-colored non-radical form (DPPH-H) in the presence of an antioxidant. The decrease in absorbance at 517 nm reflects the radical scavenging ability of the extract.

The assay is standardized against Trolox, a water-soluble analog of vitamin E, and results are expressed in % inhibition and µM Trolox equivalents (TEAC) (Brand-Williams et al, 1995; Thaipong et al., 2006). Trolox stock solution was serially diluted in methanol to obtain working standards of: 0.005, 0.01, 0.05, 0.1, 1.0, 2.0, 3.0, and 5.0 µg/mL. All solutions were freshly prepared and stored in the dark.

The *E. cardamomum* ethanolic extract was prepared at an initial concentration of 10 mg/mL, and serial dilutions were made (1, 0.5, 0.1 µg/mL) to cover a range of antioxidant activities. A1.0 mL of either extract dilution or Trolox standard was added to 5.0 mL of 0.1 mM DPPH solution in methanol in a test tube. The mixture was vortexed and incubated at room temperature (25 °C) in the dark for 30 minutes. Absorbance was recorded at 517 nm using a UV–Vis spectrophotometer. A control (DPPH + methanol only) and blank (methanol only) were used for calibration.

For each sample, % Radical Scavenging Activity:

$$\%\text{Inhibition} = \left(\frac{A_{\text{control}} - A_{\text{sample}}}{A_{\text{control}}}\right) \times 100$$

Where:

- **A control** is DPPH solution absorbance without sample.
- **A Sample** absorbance after extract or Trolox was added.

All measurements were measured in triplicates. The average and standard deviations were used for further calculations.

3.4 LC-MS/MS Analysis of Phenolic Compounds in *E. Cardamomum* extract

A Bruker Daltonik Impact II ESI-QTOF mass spectrometer and Bruker Elute UHPLC system (Bruker Daltonik GmbH, Germany, Bremen) were used to analyse *E. Cardamomum* extract phenolic compounds by LC-MS/MS. A library of authenticated standards was used to identify phenolic and flavonoid compounds by their mass-to-charge ratios (m/z) and retention times, including phenolic acids (gallic acid, trans cinnamic acid, benzoic acid, m-coumaric acid, ferulic acid, caffeic rosmarinic acid, acid, and ellagic acid) and flavonoids. For amass analyser, positive ionisation modes detected all sample components.

3.4.1 Sample preparation

The extract sample was prepared by dilution in methanol at ratio of 1:100 (v/v). Methanol was used to dissolve standards compounds into 1mg/mL stock solutions.

3.4.2 Chromatographic Conditions

- **Column:** Bruker Solo 2.0 C-18 (number of carbonsatisfactoryphase hydrophilic) UHPLC column (100 × 2.1 mm, 2.0 µm)
- **Flow rate:** 0.35 mL/min
- **Column temperature:** 40°C
- **Injection volume:** 5.0 µL
- **Mobile phases:**
- **Solvent A:** water/ Triphloroacitic acid (TFA)/formic acid (99: 0.25: 0.75)
- **Solvent B:** Acetonitrile
- **Gradient profile:** 80% to 0% B over 25 minutes, followed by washing cycle of 80% B for 8 minutes.
- **Run time:** 25 minutes in positive mode

3.4.3 Quantitative analysis for selected phenolic compounds

The quantification of caffeic acid, rutin, p-coumaric acid, and ferulic acid in the plant extract was carried out using reference authentic standards, and fixed concentrations of the plant extract.

Stock Solution Preparation: 20 mg of extract was dissolved in 200 µL of dimethyl sulfoxide (DMSO) and 1800 µL of methanol. LC-MS was used to determine each phenol content in the plant extract, based on each standard peak area prepared at concentration of (200 ng/mL), and developed under the same chromatographic conditions.

3.5 GC-MS analysis of terpenes compounds in *E. Cardamomum* extract

3.5.1 Analytical Instrumentation and Conditions

The chemical analysis employed a Shimadzu GCMS-QP 2020 system and GC-2010 gas chromatograph. Sample introduction was managed via an AOC-20i+s autosampler. To minimize cross-contamination, the syringe was cleaned using 12 rinses with presolvent and 12 rinses with post-solvent. The syringe was further conditioned with the sample twice prior to injection. Using a pumping frequency of five times and a washing volume of eight microlitres, we were able to achieve accurate volume measurements.

The temperature of the injection port was 250 °C, and it was operated in the "Normal" mode. Both the suction and injection rates of the plunger were set to "High," and the speed at which the syringe was inserted was also set to "High." In the injection port, a dwell period of 0.3 seconds was applied, and there was no terminal air gap applied.

3.5.2 Gas Chromatography Conditions

A 5.0 split ratio was used for the GC; also, helium was employed as the carrier gas at 53.5 kPa, resulting in 1.00 mL/min column flow and 36.3 cm/sec linear velocity. In addition, total flow was 7.5 mL/min, with 1.5 mL/min purge. The column oven was programmed with an initial temperature of 50.0 °C (held for 1.00 min). The temperature then increased at a rate of 10.00 °C/min to 100.0 °C (1.00 min hold), followed by a 10.00 °C/min ramp to 200.0 °C (1.00 min hold), and a final ramp of 10.00 °C/min to 280.0 °C (1.00 min hold).

3.5.3 Mass Spectrometry Detection

The mass spectrometer was run with an interface temperature of 280.00 °C and an ion source temperature of 230.00 °C. To safeguard the detector, a solvent cut time of two minutes was put in place. The detector gain was set relative to the tuning result at 0.89 kV + 0.50 kV. Data acquisition was conducted in Scan mode from 2.00 to 27.00 minutes.

The mass-to-charge (m/z) ratio was scanned from 50.00 to 650.00. The event time was 0.30 seconds with a scan speed of 2500.

3.6 Antimicrobial Activity: Determination of MIC and Minimum Bactericidal Concentration (MBC)

The MIC was determined following the method reported by (Abu Ershaid J.M, et al, 2024; Aboulwafa M.M.et al, 2025) using a 96-well plate test. In brief, 100 µL of nutrient broth was added to each well for *B. cereus, S. aureus*, *E. coli,* and *P. aeruginosa*. Then, 100 µL of cardamom extract (that showed antimicrobial activity on each bacterium) were separately added to the first well and serially diluted to the following concentrations: 100, 50, 25, 25, 12.5, 6.25, 3.125, 1.562, 0.781, 0.391, 0.195, 0.098, and 0.049 mg/mL. Then, 100 µL of bacterial suspension (1×10^6 CFU/mL) was added in each well. For a period of 18 hours, the plates were kept in an incubator at 37° Celsius. For the purpose of determining the MIC, the lowest concentration at which there was no obvious development of bacteria was used.

Subculturing 15 µL of MIC broth wells that showed no growth onto nutrient agar plates allowed for the determination of the MBC. The minimum concentration required to eradicate the bacteria was known as the MBC (Aboulwafa et al., 2025).

3.7 Tyrosinase and collagenase inhibition assay: in silico studies

3.7.1 Protein Preparation

The crystal structure of the human collagenase catalytic domain was obtained from the Protein Data Bank (PDB), and selected based on its suitable resolution for docking studies (PDB ID: 1CGL; 2.4 Å), which includes a co-crystallized inhibitor bound within the catalytic site, supporting accurate active-site localization and structural reliability for silico modeling.

Because no experimentally determined human tyrosinase structure meeting docking requirements was available in the PDB, a validated homology-guided approach was adopted following the protocol reported by Jarrar et al. (2025). Briefly, the predicted structure of human tyrosinase (UniProt: P14679) was retrieved from the AlphaFold Protein Structure Database (AlphaFold code: AF-P14679-F1-model_v6). To confirm the catalytically relevant binding pocket, the AlphaFold model was superimposed onto a

ligand-bound template structure (PDB ID: 6JU7), which is co-crystallized with L-tyrosine, using the "superimpose by sequence alignment" method in BIOVIA Discovery Studio 16, enabling precise identification of the native active site.

Both protein structures were subsequently prepared for molecular docking in SAMSON Integrative Molecular Design (version 2025 R3, 10.0.0). During preparation, crystallographic water molecules, solvents, ions, and other non-essential heteroatoms were removed, followed by the addition of hydrogen atoms and the assignment of partial charges to generate energetically consistent and simulation-ready receptor models.

3.7.2 Ligands Preparation

All four ligands (p-Commaric acid, Rutin, Caffeic acid, and Ferulic Acid) were obtained from PubChem (https://pubchem.ncbi.nlm.nih.gov/) as a 3D conformer. Using the Universal Force Field (UFF) in the Avogadro 1.2.0 software, all of the compounds were minimised, and then they were uploaded to SAMSON Integrative Molecular Design. This allowed the compounds to be produced by adding hydrogens and charges, as well as generating three-dimensional conformers for molecular docking.

3.7.3 Docking Simulation

The extended AutoDock Vina wizard included in SAMSON Integrative Molecular Design was used to carry out molecular docking. The docking grid-box was automatically generated, and its dimensions were defined as 20 × 20 × 20 Å to adequately encompass the catalytic binding pockets of the target enzymes. Docking poses were evaluated based on the lowest estimated binding energy (LEB) to identify the most energetically favorable ligand–receptor conformations. Software for adaptive modelling and simulation of nano-object (SAMSON) was used to visualize the top-ranked complexes and 2D interaction diagrams were used to characterize active site intermolecular interactions.

3.8 Statistical Analysis

Version 25 of the Statistical Package for the Social Sciences (SPSS) was utilized in order to carry out analytical statistical procedures. Also, it was necessary to do each experiment three times. The data were reported in the form of the mean ± the standard deviation.

Through the utilization of the One-way Analysis of Variance (ANOVA), it was possible to ascertain whether or not there were noteworthy distinctions between the groups. Following the conduct of the analysis of variance (ANOVA), the application of Tukey's post hoc test was carried out in order to ascertain which specific groups display statistically significant differences. It was determined that a statistically significant result was achieved when the P-value was less than 0.05.

Chapter Four

Results of the Study

This chapter presents Elettaria cardamomum seed ethanolic extract experimental and analytical results. Results are organised systematically according to objectives and methodology from previous chapters, allowing a clear progression from phytochemical characterisation to biological activity evaluation and molecular interaction analysis. Extraction yield, phytochemical screening, total phenolic and total flavonoid contents, and DPPH radical scavenging assay antioxidant activity are discussed in the chapter. These results provide the chemical and functional foundation for biological evaluations.

In addition, advanced chromatographic analyses using LC-MS/MS and GC-MS identify and quantify the major phenolic and terpenoid compounds in the E. cardamomum ethanolic extract. These analyses reveal the chemical composition and bioactive constituents that cause biological effects. MIC and MBC against Staphylococcus aureus demonstrate the extract's antibacterial potential. In silico molecular docking studies of selected phenolic compounds' collagenase and tyrosinase enzyme binding affinity and interaction profiles reveal their inhibitory potential.

4.1 Extraction Yield

The following formula was used to calculate E. cardamomum ethanolic extract yield.

- Extract weight (W_e) = 60 g
- Plant material used (W_p) = 2 kg
- Extraction Yield (%) = 3%

This indicates moderate extraction efficiency using ethanol maceration method.

4.2 Phytochemical Screening

4.2.1 Determination of Total Phenolic Content

A calibration curve was constructed for gallic acid standards as shown in Figure 4.1. The linear regression equation was: y = 0.0093x + 0.0105.

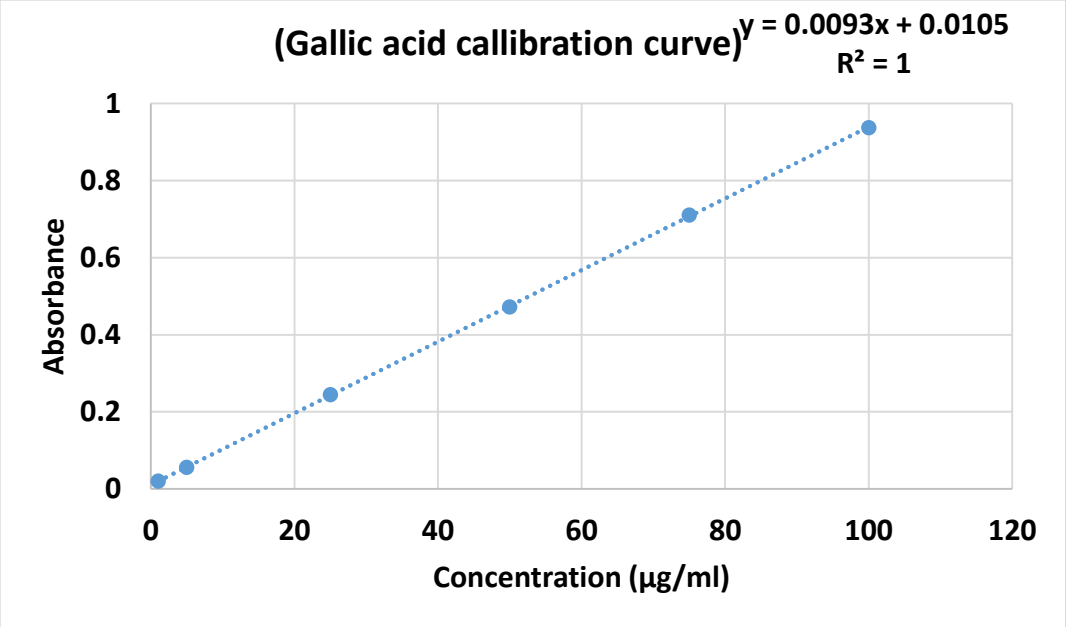


Figure 4.1: Gallic acid calibration curve.

Absorbance data for the plant extract were translated into GAE concentrations by using the regression equation that was presented earlier. The total phenolic content was calculated as **(1.78 mg equivalent GAE / g (dry plant extract)**, indicating a relatively high content of polyphenolic compounds in the prepared extract.

4.2.2. Total flavonoid content

A calibration curve was developed for quercetin standards, and it is depicted in Figure 4.2 to illustrate this. The equation for linear regression was as follows:

$$y = 0.0025x + 0.0102.$$

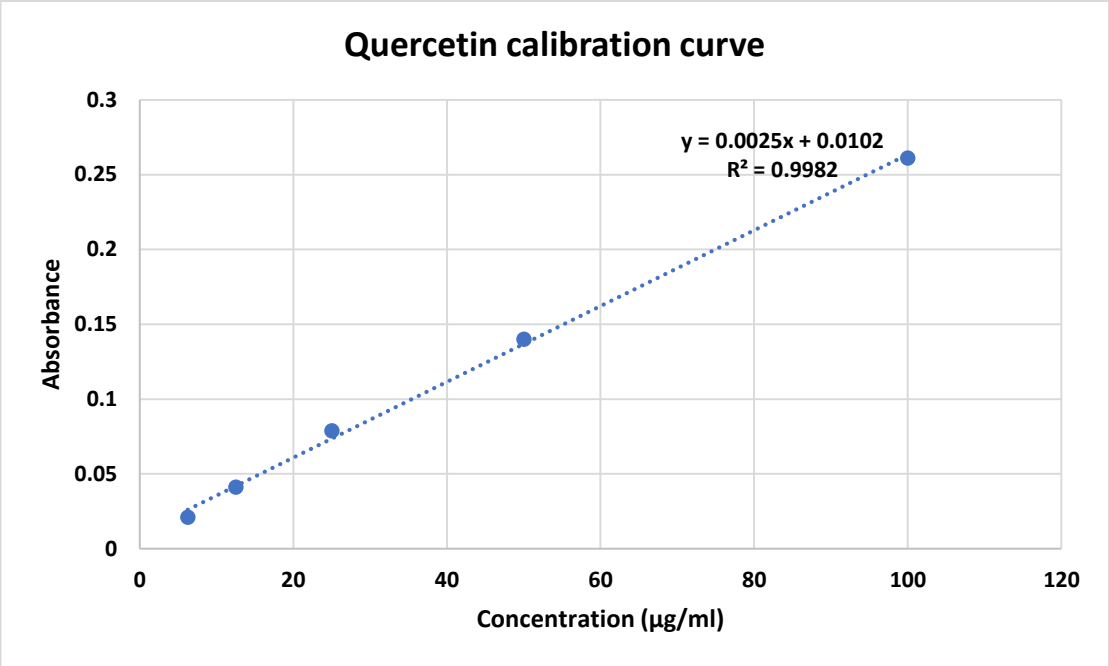


Figure 4.2: Calibration curve of Quercetin.

The regression equation above transformed plant extract absorbance values into quercetin concentrations. A rather high concentration of flavonoid components was found in the produced extract, as indicated by the fact that the total flavonoid content was assessed to be 0.3 mg equivalent quercetin per gramme of dry plant extract used.

4.2.2 Determination of Antioxidant Activity (DPPH Assay)

Findings of Trolox DPPH assay show a consistent decline in absorbance as Trolox concentration increases, indicating a dose-dependent antioxidant activity. A standard calibration curve was constructed based on the absorbance reduction of Trolox solutions at known concentrations, as illustrated in Figure (4.3).

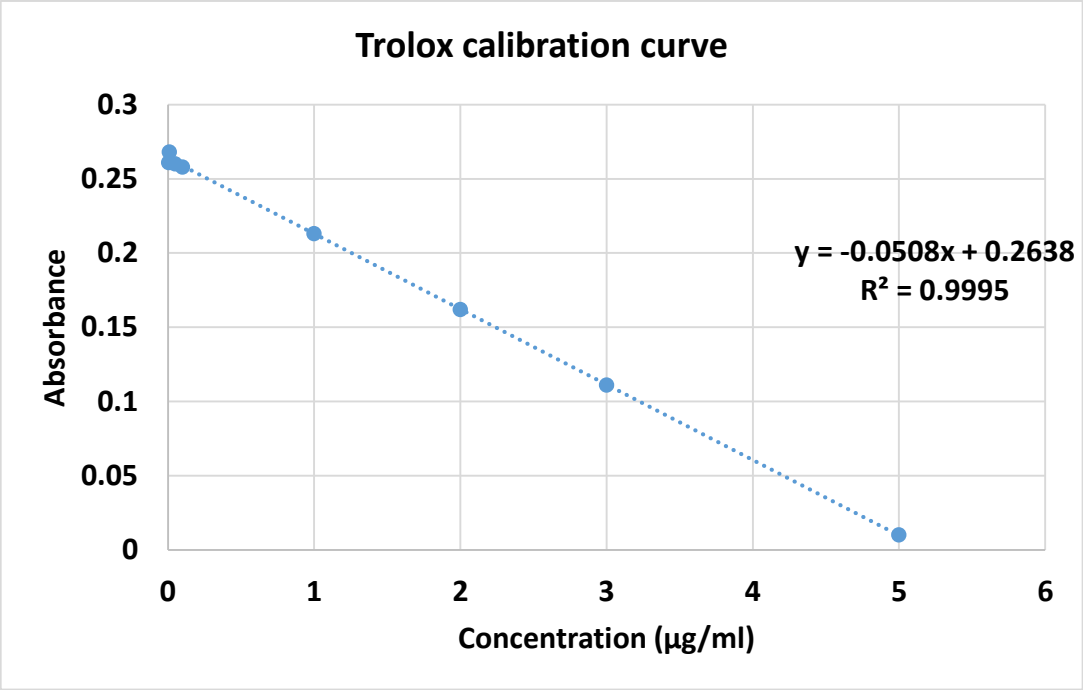


Figure 4.3: Calibration curve of Trolox.

A linear regression equation for Trolox standards calibration curve was obtained:

$$y = –0.0508x + 0.2638.$$

This formula was applied to determine the extract's antioxidant capacity in relation to Trolox (TEAC), in triplicate and reported as (mean ± SD). Results showed that *cardamom* extract exhibited dose-dependent antioxidant activity, with maximum activity observed at (**0.04 mg/ g).**

4.3 LC/MS-MS analysis of phenolic compounds in *E. Cardamomum* extract

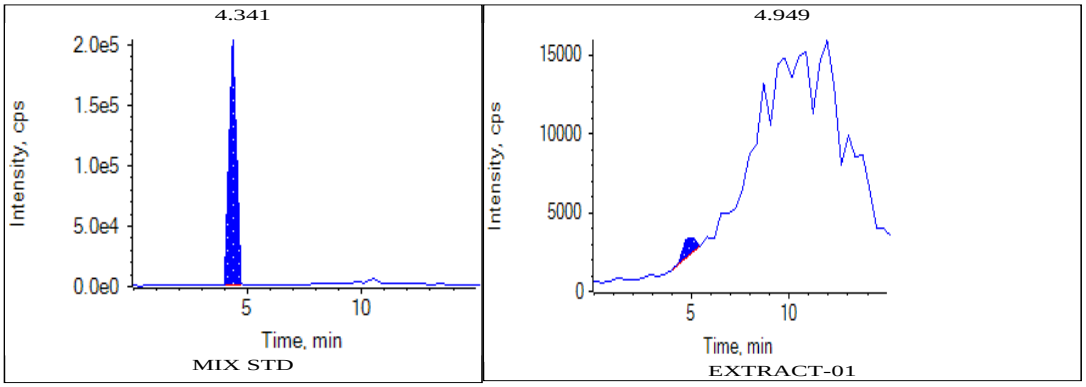
4.3.1 Phenolic compounds detected using Positive Ion Mode

Findings revealed the presence of P-commaric acid, Rutin, caffic acid and Ferulic Acid, were detected in the *E. cardamomum* extract based on their RT values as shown in their chromatograms (Figure 4. 4) .

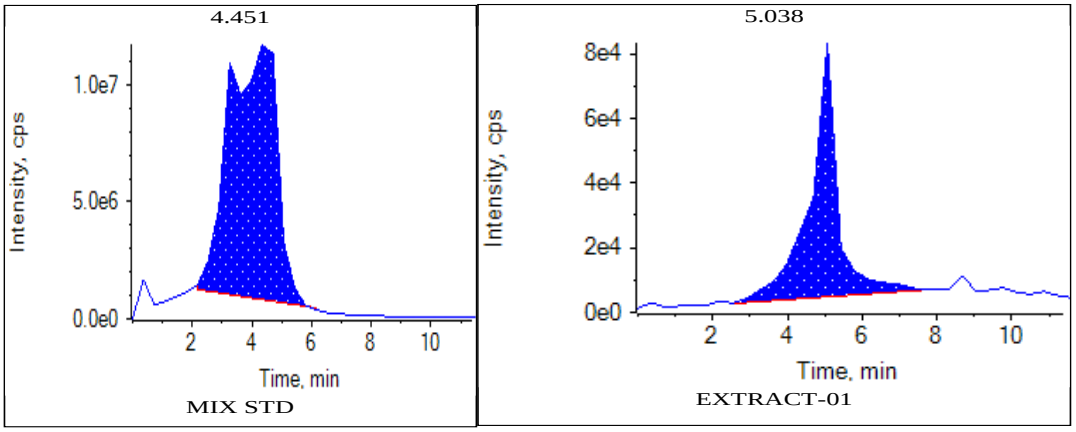
Of these four detected major phenolic compounds, their peak intensity was converted into relative concentrations (relative to standard peak area) as shown in Table (4.1).

Findings revealed that P-coumaric acid was the most abundant, followed by caffeic acid and Ferulic Acid, Rutin was found in trace amount in this prepared extract.

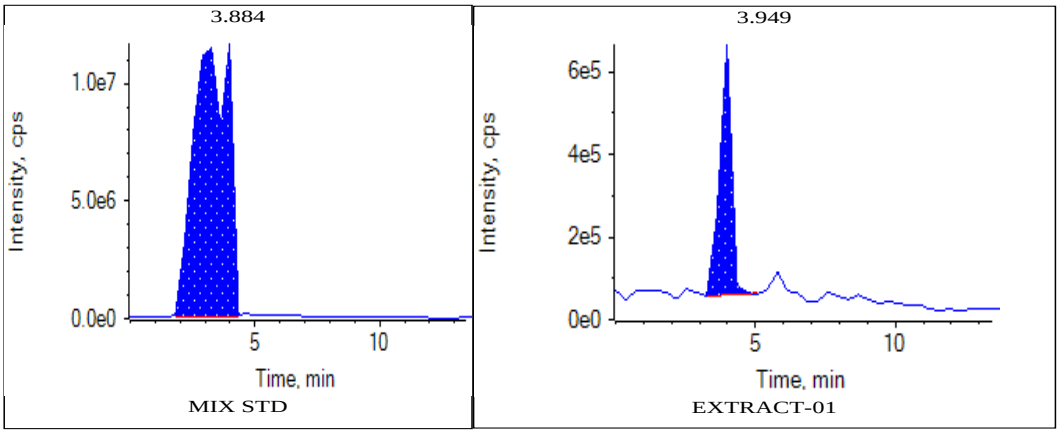
CAFFIC ACID



RUTIN



P-COMMARIC ACID



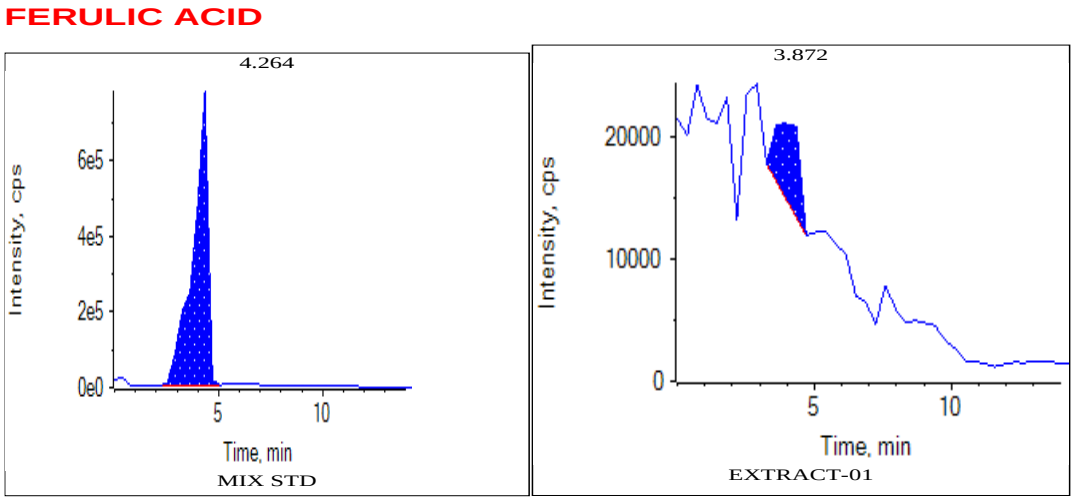


Figure 4.4: LC Chromatograms for the major phenolic compounds (standard and plant extracted) detected in the E. cardamomum extract based on their RT.

Table 4.1: Major phenolic Compounds content in the E. cardamomum extract determined using LC analysis.

Phenolic compound	Type	Analyte peak area * (counts)	RT (min)	Concentration (µg/ ml)
P-coumaric acid	Standard	1151508277	3.884	--
	Extract	17709295	3.949	3.075843
Rutin	Standard	1251411580	4.451	--
	Extract	4043222	5.038	0.646186
Caffeic acid	Standard	4427968	4.341	--
	Extract	49145	4.949	2.219754
Ferulic Acid	Standard	39102745	4.264	--
	Extract	398661	3.872	2.039044

* These results indicate the presence of compounds and are relative quantitative content depending on the in-house developed library (concentration of corresponding standard stock solution 200 (µg/ ml).

4.4 GC-MS analysis

Identification of the different compounds found in E. cardamomum ethanolic extracts, using GC analysis, are shown in (Figure 4.5, and Table 4.2).

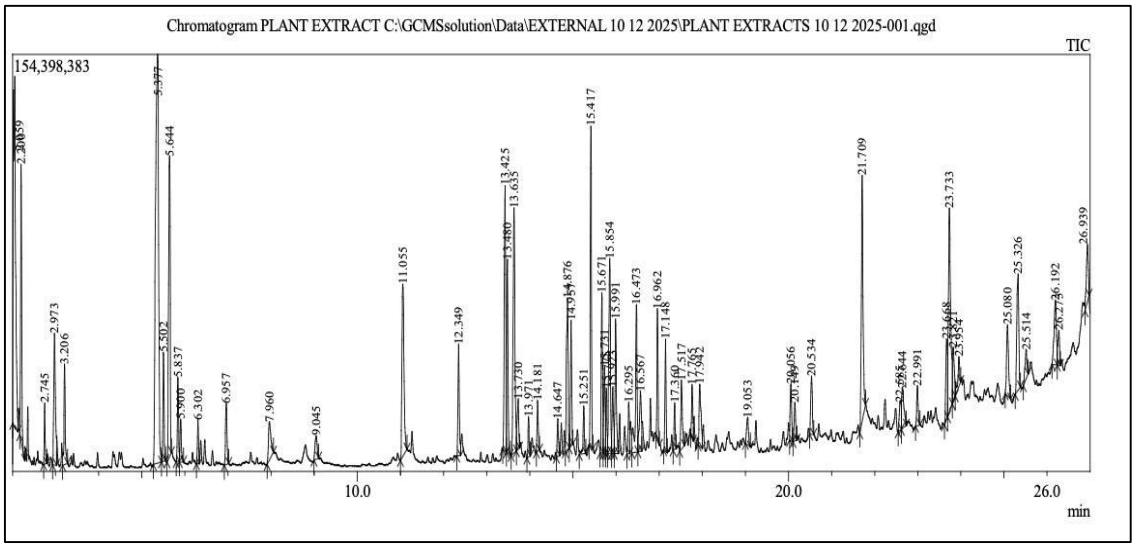


Figure 4.5: GC chromatogram for compounds detected in the E. cardamomum ethanolic extracts.

Table 4.2: GC analysis of different compounds identified in the E. cardamomum ethanolic extract.

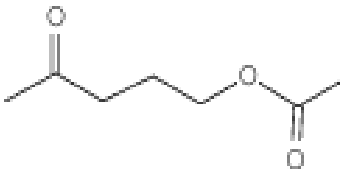
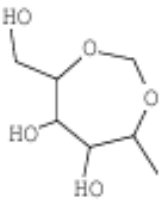
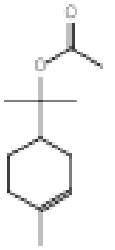
Peak#	R.Time	Area%	Name
1	2.059	7.22	1,3-Dioxolane, 4-methyl-2-(2-methylpropyl)
2	2.2	2.75	Oxirane, 2,2'-(1,4-butanediyl)bis-
3	2.745	0.52	Tetrahydrofuran, 2,2-dimethyl
4	2.973	2.01	3-Heptanol
5	3.206	1.12	3-Pentanol, 2,3-dimethyl-
6	5.377	11.15	2-Pentanone, 5-(acetyloxy)-
7	5.502	1.17	Pentanoic acid, 2-propenyl ester
8	5.644	4.48	2,5-Monomethylene-l-rhamnitol
9	5.837	0.91	1,2,6-Hexanetriol
10	5.9	0.5	Allyl isovalerate
11	6.302	0.46	Benzene, 1-ethyl-4-methyl-
12	6.957	0.83	Mesitylene
13	7.96	0.88	2,5-Dihydroxybenzaldehyde, 2TMS derivate
14	9.045	0.45	Cyclotetrasiloxane, octamethyl-
15	11.055	3.3	1,3,5-Benzetriol, 3TMS derivative
16	12.349	1.34	Cyclopentasiloxane, decamethyl-
17	13.425	3.79	.alpha.-Terpinyl acetate
18	13.48	2.24	Dodecanedioic acid, 2TBDMS derivative
19	13.635	4.11	1,3,5-Benzetriol, 3TMS derivative

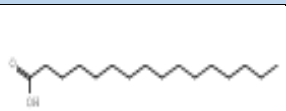
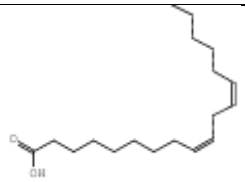
Peak#	R.Time	Area%	Name
20	13.73	0.74	Hexasiloxane, tetradecamethyl-
21	13.971	0.41	Cyclohexasiloxane, dodecamethyl
22	14.181	0.54	Dodecanedioic acid, 2TBDMS derivative
23	14.647	0.45	Cycloheptasiloxane, tetradecamethyl-
24	14.876	2.37	Cycloheptasiloxane, tetradecamethyl-
25	14.957	1.4	Cycloheptasiloxane, tetradecamethyl-
26	15.251	0.55	Cycloheptasiloxane, tetradecamethyl-
27	15.417	3.47	Cyclononasiloxane, octadecamethyl-
28	15.671	1.85	Dodecanedioic acid, 2TBDMS derivative
29	15.731	1.03	Dodecanedioic acid, 2TBDMS derivative
30	15.775	0.71	Dodecanedioic acid, 2TBDMS derivative
31	15.854	2.98	Cyclooctasiloxane, hexadecamethyl-
32	15.923	0.9	Cyclooctasiloxane, hexadecamethyl-
33	15.991	1.73	Heptasiloxane, hexadecamethyl-
34	16.295	0.62	Citric acid, 4TBDMS derivative
35	16.473	2.31	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (
36	16.567	1.12	8-Hydroxycarvotanacetone
37	16.962	1.23	Cyclooctasiloxane, hexadecamethyl-
38	17.148	1.16	Cyclooctasiloxane, hexadecamethyl-
39	17.360	0.46	Cycloheptasiloxane, tetradecamethyl-
40	17.517	0.96	Cycloheptasiloxane, tetradecamethyl-
41	17.765	0.6	Cyclooctasiloxane, hexadecamethyl-
42	17.942	1.07	Cyclooctasiloxane, hexadecamethyl-
43	19.053	0.48	Cyclononasiloxane, octadecamethyl-
44	20.056	0.74	1-Naphthalenepropanol, .alpha.-ethenyldeca
45	20.149	0.49	Pentadecanal-
46	20.534	0.86	1,2-Benzenedicarboxylic acid, bis(2-methylp
47	21.709	3.87	n-Hexadecanoic acid
48	22.585	0.54	Tetracosane
49	22.644	0.84	Tetracontane
50	22.991	0.55	Phenanthrene, 7-ethenyl-
51	23.668	1.17	9,12-Octadecadienoic acid
52	23.733	4.28	9-Octadecenoic acid
53	23.821	0.9	Dihydrotachysterol

Peak#	R.Time	Area%	Name
54	23.954	0.51	Octadecanoic acid
55	25.08	1.27	Dotriacontane
56	25.326	2.14	Pentatriacontane
57	25.514	0.53	Cyclononasiloxane, octadecamethyl-
58	26.192	1.39	1-Naphthalenepropanol, .alpha.-ethenyldeca
59	26.273	0.53	Tetracosane
60	26.939	1.04	Octadecane, 3-ethyl-5-(2-ethylbutyl)-

Chromatograms obtained from the GC-MS analysis for *E. cardamomum* extract revealed the presence of 5 major secondary metabolites. The GC-MS chromatogram identified the major compounds are shown in (Appendix 1). Table (4. 3) show the structures of these major compounds identified in *E. cardamomum* extract using GC-MS analysis. Findings revealed the presence of terpenoid esters, fatty acids, and oxygenated volatile-derived compounds. α-Terpinyl acetate was identified as a characteristic aromatic constituent (Masyita et al., 2022)

Table 4.3: Structures of the major compounds identified in E. cardamomum extract using GC-MS analysis.

Peak	R time	Area%	Name/ class	Structure
6	5.377	11.15	2-Pentanone, 5-(acetyloxy) Oxygenated ketone volatiles	
8	5.644	4.48	2,5-Monomethylene-l-rhamnitol Monoterpene ester	
17	13.425	3.79	A-Terpinyl acetate Terpenoids	

Peak	R time	Area%	Name/ class	Structure
47	21.709	3.87	n-Hexadecanoic acid Saturated fatty acids	
52	23.733	4.28	9-Octadecenoic acid Unsaturated fatty acids	

4.5 Antimicrobial Activity

The ethanolic extract of E. cardamomum was tested for its antimicrobial activity against *Staphylococcus* aureus and other gram-positive bacteria. The extracts were effective against the Gram-positive bacteria at all concentrations. Therefore, MIC and MBC values for the extract were measured at concentration of **(0.049 mg/g).**

4.6 Results of Tyrosinase and collagenase inhibition: in silico tests

Molecular docking of caffeic acid, ferulic acid, *p*-coumaric acid, and rutin against human tyrosinase (AlphaFold model: AF-P14679-F1-model_v6) and human collagenase (PDB ID: 1CGL) yielded stable binding poses confined within the catalytic pockets defined by a 20 × 20 × 20 Å grid box. Ligand affinity was ranked according to the (LEB, kcal·mol^{-1}), and the top-ranked complexes were further notanalyzed for key intermolecular interactions using SAMSON Integrative Molecular Design.

4.6.1 Binding Affinity Overview

For tyrosinase, docking scores ranged from **−4.765 to −6.842 kcal·mol^{-1}**, with **caffeic acid presenting the strongest predicted affinity (−6.842 kcal·mol^{-1})**, followed by *p*-coumaric acid (−6.708 kcal·mol^{-1}), ferulic acid (−6.631 kcal·mol^{-1}), and rutin (−4.765 kcal·mol^{-1}). For collagenase, binding energies ranged from **−6.82 to −8.425 kcal·mol^{-1}**, with **rutin showing the most favorable score (−8.425 kcal·mol^{-1})**, followed by caffeic acid (−7.217 kcal·mol^{-1}), *p*-coumaric acid (−7.007 kcal·mol^{-1}), and ferulic acid (−6.82 kcal·mol^{-1}) table 1 summarize the interactions between each ligand and the targeted proteins.

4.6.2 Tyrosinase Interaction Profile

- Caffeic acid (LEB: −6.842 kcal·mol⁻¹) formed two conventional hydrogen bonds with GLN 90 and GLY 93, without additional non-bonded interactions reported.
- Ferulic acid (LEB: −6.631 kcal·mol⁻¹) established hydrogen bonds with GLN 90 and GLY 93, further supported by one polar contact with SER 92.
- *p*-Coumaric acid (LEB: −6.708 kcal·mol⁻¹) exhibited the richest interaction network, forming six hydrogen bonds with HIS 180, HIS 202, ARG 308, HIS 363, SER 380, and HIS 390, and additional stabilization via π–π stacking with PHE 347, polar contact with ASN 364, and hydrophobic interactions with VAL 377 and PHE 347.
- Rutin (LEB: −4.765 kcal·mol⁻¹) formed three hydrogen bonds with GLN 56, ASN 94, and LYS 104, and a secondary stabilization network involving polar interactions with SER 92 and GLY 93.

4.6.3 Collagenase Interaction Profile

- Rutin (LEB: −8.425 kcal·mol⁻¹) produced the most stable collagenase complex, forming five hydrogen bonds with ASN 180, LEU 181, ALA 182, ARG 214, and HIS 218, along with additional hydrophobic and van der Waals stabilization mediated by PRO 238, SER 239, and TYR 240. Rutin also formed two polar contacts with SER 92 and GLY 93 outside the zinc center, further promoting complex stability.
- Caffeic acid (LEB: −7.217 kcal·mol⁻¹) formed five hydrogen bonds with ASN 180, LEU 181, ALA 182, ARG 214, and HIS 218, and its complex was stabilized by aromatic and polar contacts with TYR 237, PRO 238, and SER 239.
- Ferulic acid (LEB: −6.82 kcal·mol⁻¹) formed five hydrogen bonds with ASN 180, LEU 181, ALA 182, ARG 214, and HIS 218, and exhibited hydrophobic interactions with TYR 237 and polar contact with SER 239.
- *p*-Coumaric acid (LEB: −7.007 kcal·mol⁻¹) formed five hydrogen bonds with ASN 180, LEU 181, ALA 182, ARG 214, and HIS 218, and showed further stabilization through hydrophobic and polar contacts involving PRO 238, SER 239, and TYR 240.

Table 4. 4: Analysis of all ligand molecular docking simulations showing amino acid residue binding.

	Tyrosinase		Collagenase	
	H-bond	**other interactions**	**H-bond**	**other interactions**
Caffeic_Acid	GLN 90, GLY 93	N/A	ASN 180, LEU 181, ALA 182, ARG 214, HIS 218	TYR 237, PRO 238, SER 239
Ferulic_Acid	GLN 90, GLY 93	SER 92		TYR 237, SER 239
P-Coumaric_Acid	HIS 180, HIS 202, ARG 308, HIS 363, SER 380, HIS 390	PHE 347, ASN 364, VAL 377		PRO 238, SER 239, TYR 240
Rutin	GLN 56, ASN 94, LYS 104	SER 92, GLY 93	ASN 180, LEU 181, ALA 182, ARG 214, HIS 218, HIS 222, HIS 228	

4.6.4 Mechanistic Relevance and Structural Validity

All ligands bound within catalytically relevant regions without steric clashes or geometric distortion, supporting the robustness of the receptor and ligand preparation workflow. The high hydrogen-bond multiplicity observed for ***p*-coumaric acid in tyrosinase** is consistent with competitive active-site engagement by small phenolic scaffolds, whereas **rutin demonstrated superior confinement and interaction cooperativity in collagenase**, reflecting the highest predicted stability among all tested complexes. Collectively, these findings nominate **caffeic acid as the top tyrosinase binder by energy**, and **rutin as the most promising collagenase inhibitor candidate**, warranting further validation using molecular dynamics and binding free-energy calculations. (Figures 4.6 and 4. 7 show the 2D interactions between the ligands and the proteins).

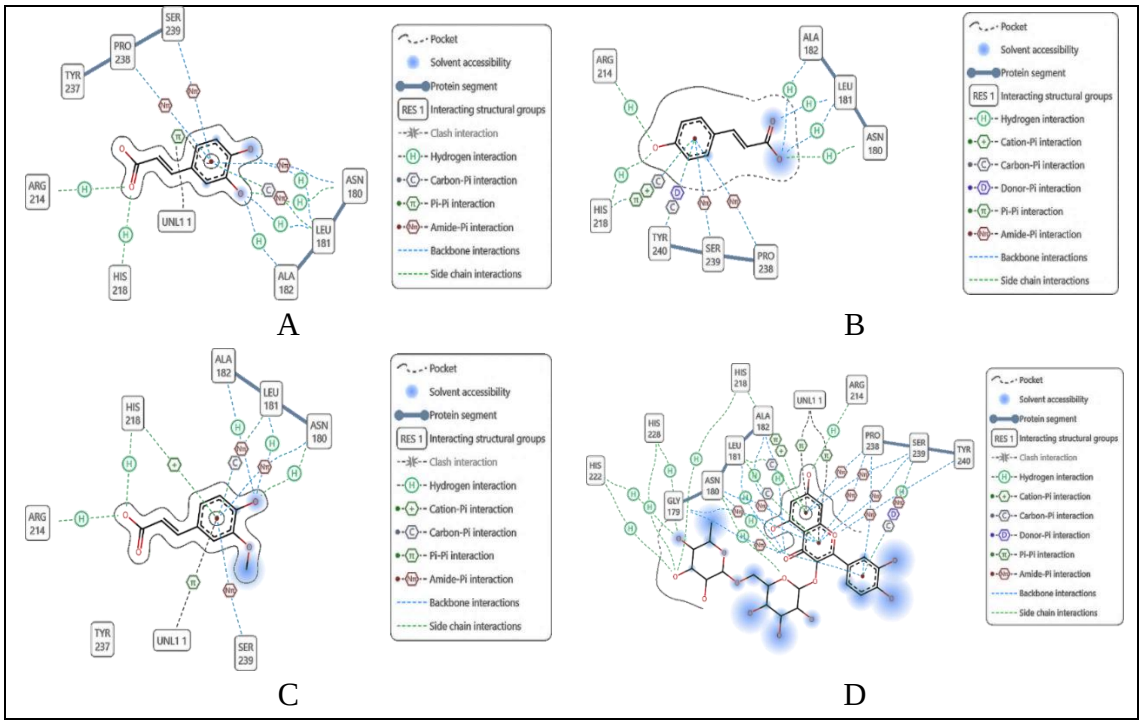


Figure 4. 6: 2D representation of the interaction between ligands and the collagenase protein where A: caffeic acid, B: p-coumaric acid, C: ferulic acid, D: rutin

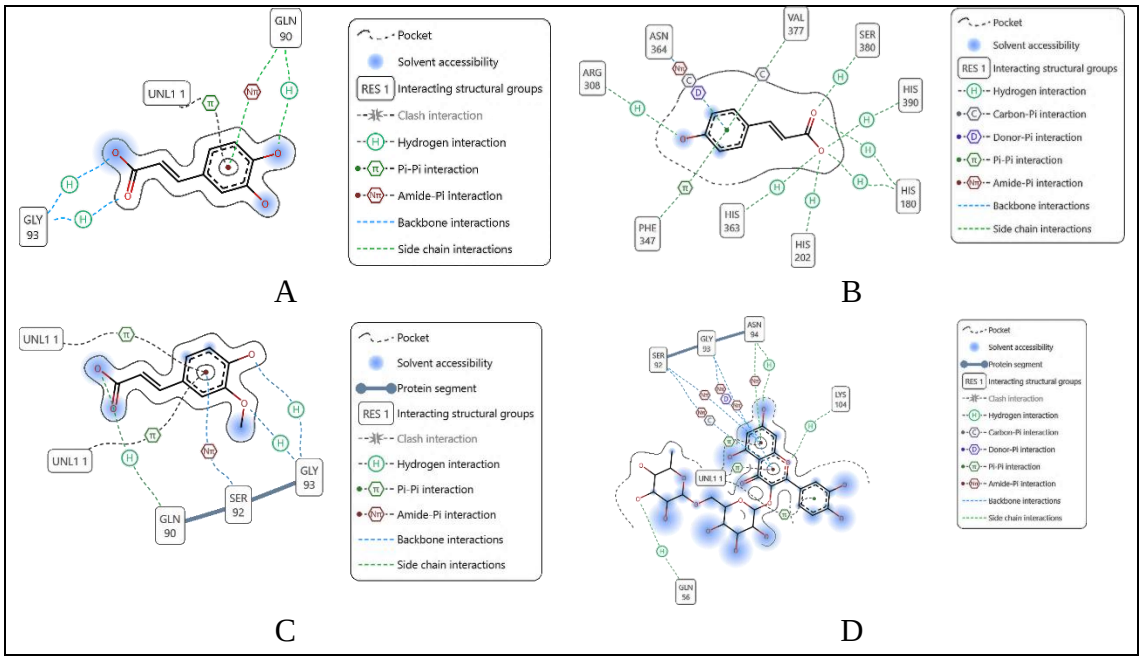


Figure 4.7: 2D representation of the interaction between ligands and the tyrosinase protein where A: caffeic acid, B: p-coumaric acid, C: ferulic acid, D: rutin

Chapter Five

Discussion of Findings and Recommendation

Asthma, gum infections, cataracts, intestinal, renal, and heart disorders have been treated with cardamom. Aghasi et al. (2018) also found anticancer, hypoglycemic, antioxidant, and anti-inflammatory properties. Also, plants produce most polyphenols, which are naturally occurring compounds with phenolic properties (Singla et al., 2019). This research focusses on E. cardamomum extract flavonoids and phenolic acids. In addition, Abbas et al. (2017) state that these two primary polyphenol groups have several biological actions and are essential in fighting many diseases.

The seeds, skin, and whole cardamom extracts were previously utilized to calculate the overall phenolic content, which was 124.5, 71.7, and 141.5 mg phenolics/100 g. Sowmya and Narendhirakannan (2025) report a total flavonoid concentration of 45.5 µg/mL in the aqueous extract of E. cardamomum. Total phenolic and flavonoid content of the current study was 1.78 mg equivalent GAE/g (dry plant extract) and 0.3 mg equivalent quercetin/g. These findings indicated that the extract includes a lot of polyphenolic and flavonoid compounds.

Findings of this study investigating the phytochemical composition of *E. cardamomum* extract using GC-MS analysis, revealed the presence of terpenoid esters, fatty acids, and oxygenated volatile-derived compounds. A unique aromatic ingredient, α-Terpinyl acetate, was found in the extract, along with other lipid-based components.

p-coumaric acid, rutin, caffeic acid, and ferulic acid were identified as major phenolic compounds in the extract of E. cardamomum, according to the results of an LC-MS investigation. These findings are consistent with the polyphenol profile of whole cardamom, peel, and seeds that was published by Sreedharan et al. (2023). For the first time, they discovered eleven phenolic compounds in whole cardamom, peel, and seeds. These chemicals included rutin, syringic acid, 5-O-caffeoylquinic acid, sinapoyl quinic acid, and feruloyl quinic acid. The following acids are also included in the category of cardamom phenolics: protocatechuic acid, gentisic acid, vanillic acid, caffeic acid, p-coumaric acid, and ferulic acid (Variyar et al., 1995). Hong et al. (2015) and Beltran-Ramirez et al. (2008) found caffeic acid, gallic acid, and 4,5-dicaffeoyl quinic acid in cardamom seed. In addition, Elguindy et al. (2016) found gallic acid, tannic acid, caffeic

acid, and 4.5-dicaffeoyl quinic acid in HPLC/UV-analyzed cardamom extract. Further, Rahman et al. (2017) stated that the ethanolic extract of cardamom contains: vanillin, epicatechin, p-coumaric acid, trans-ferulic acid and ellagic acid.

Caffeic acid, as a result, demonstrates immunomodulatory and anti-inflammatory activity, in addition to being an antioxidant both in vitro and out in the wild. In comparison to other antioxidants, caffeic acid demonstrated superior performance, resulting in a reduction in aflatoxin formation by more than 95 % (Olthof et al., 2001). It has been shown that ferulic acid can be present in Chinese medicinal herbs such as Ligusticum chuangxiong, Cimicifuga heracleifolia, and Angelica sinensis (often known as female ginseng). There is also evidence of its presence in the tea that was prepared from the European century (Centaurium erythraea), which is a plant that is utilised as a medicinal herb in several regions of Europe (Valentao et al., 2001).

In wine, the yeast Brettanomyces is responsible for the production of p-coumaric acid, which is the precursor of 4-ethylphenol. Through the action of the enzyme cinnamate decarboxylase, the yeast is able to transform this into 4-vinylphenol. The enzyme known as vinyl phenol reductase is responsible for the further reduction of the compound 4-vinylphenol to 4-ethylphenol. According to Cynkar et al. (2007), the incorporation of coumaric acid into microbiological media has the potential to occasionally make it possible to positively identify Brettanomyces by the utilization of our sense of smell.

In Turkey, Goze et al. (2009) tested Origanum rotundifolium Boiss essential oil and extracts for antioxidant activity, supporting this idea. This study found that extract constituents had antioxidant and antibacterial properties. Geography, temperatures, plant development phase, harvest duration, plant, soil element, and plant-related environmental and genetic variables also affected these activities.

The findings of the current study illustrated the health advantages of plant extract; the aqueous extract also exhibited significant antibacterial activity against the tested bacterial strain of our results, suggesting it could be used to treat some pathogenic infections. Also, E. cardamomum ethanol extract was tested against S.aureus. In addition, MIC and MBC were tested at 0.049 mg/g extract concentration. Toxicity, biochemical, and histological tests of E. cardamomum's antibacterial activity by El Malti et al. (2007) accord with these results. The minimum inhibitory concentration (MIC) of the cardamom

extract varied from (9.4 to 18.75) mg/mL for all organisms except E. coli, Bacillus cereus, and Enterobacter cloacae, which were exceedingly sensitive.

In antimicrobial experiments, Sowmya and Narendhirakannan (2025) found effective inhibition of Gram-positive and Gram-negative bacteria, with an 18 mm zone of inhibition against P. aeruginosa at 100 µg/mL. Additionally, Moulai-Hacene et al. (2020) examined the chemical composition and antibacterial activities of E. cardamomum extract. They compared the antibacterial properties of 10 harmful bacteria types. The research also showed that the plant extract was antibacterial against all microbes. In conclusion, this substance's potent inhibitory effect comes from its high phenolic content. Similarly, Mutlu-Ingok et al. (2017) discovered that cardamom essential oils were more antimicrobial than cumin. The research found that cardamom essential oils had bigger inhibition zones and lower inhibition thresholds than Campylobacter jejuni and coli. The study also examined antibacterial systems.

The antibacterial activity of E. cardamomum fruit extracts was also investigated from the perspective of oral microorganisms. Aneja et al. (2009) found that the most significant effect was on S. aureus, and that the extracts of the substance in ethanol and acetone may have antibacterial properties. The results of this investigation supported the findings of Arora and Kaur (2007), who discovered that the aqueous extract of E. cardamomum inhibited a variety of pathogenic bacteria in inhibition zones ranging from 15 to 28 *millimetres.* Also, Nanasombat and Lohasuthawee (2025) examined the antibacterial activity of crude ethanolic extracts and spice essential oils against Salmonella and other enterobacteria. However, all cultures examined revealed a 7–12 mm inhibitory zone from cardamom seed ethanolic extract.

The aqueous extract of cardamomum extract, on the other hand, was found to have no antibacterial activity in a study that was carried out in India for the purpose of screening some Indian medicinal plants for their antimicrobial properties. This was discovered to be the case due to either the extraction method or strain differences (Ahmad et al., 2014).

It is possible that the phenolic chemicals found in the plant extract are responsible for the antibacterial activity that it possesses. When these substances are present, they have the ability to increase permeability and destroy cytoplasmic content by targeting the phospholipids that

are found in the cell membrane. Moreover, these substances have the potential to influence the enzymes that are found in the bacterial cell walls (Wu et al. 2013, 2014).

According to Mukattash et al. (2024), it has been demonstrated that phenolic acids inhibit the activity of tyrosinase in a manner that is competitive. Molecular docking simulations were carried out in order to analyse the inhibitory effects of four phenolic compounds known as caffeic acid, ferulic acids, p-coumaric acids, and rutin. These simulations were carried out with the use of high-resolution crystal structures (PDB ID: 1CGL) and validated AlphaFold models (AF-P14679-F1-model_v6). Both human tyrosinase and collagenase were put through resistance testing with these substances. A study conducted by (Pradiba and colleagues ,2018) discovered that docking guaranteed an accurate active site image and a reliable interpretation of ligand-enzyme interactions.

A considerable body of research has focused on the inhibition of tyrosinase by natural compounds (Kim & Uyama, 2005). Previous studies have demonstrated that hydroxycinnamic acids positively interact with the active sites of tyrosinase (Yu and Fan, 2021; Zolghadri et al., 2019; Mukattash et al., 2024). Caffeic acid performed reasonably well in binding among the tested ligands, with an LEB of -6.842 kcal·mol^{-1}. Ferulic and chlorogenic acids have high binding affinities and competitive inhibition of human tyrosinase activity, with binding energies from (-6.8 to -7.2) kcal·mol^{-1} and competitive inhibition observed in biochemical assays (Yu and Fan, 2021). This concordance supports the validity of the observed affinity for caffeic acid in our tyrosinase model.

Contrary to overall binding energy, p-coumaric acid formed an extensive interaction network within the tyrosinase active site, establishing six hydrogen bonds with residues including HIS180 & HIS202, as well as (π–π) stacking with PHE347. Literature on structurally related hydroxycinnamic acids (Yu and Fan, 2021), suggests that such extensive hydrogen bonding and aromatic contacts enhance enzyme recognition and may contribute to inhibitory efficacy even when global binding energy differences are modest.

In addition, ferulic acid was not the strongest binder in this docking set, but studies have shown that it allosterically interacts with tyrosinase and modulates conformation at physiologically relevant amounts, supporting its role in melanin suppression in cellular models (Alkhadhrh et al., 2024). This docking data confirms biological trends for compounds of hydroxycinnamic acid.

For collagenase, rutin had the strongest binding affinity, with a lower energy binding (LEB) of -8.425 kcal·mol^{-1}; it is much greater than the other phenolic ligands studied. The cooperative network of noncovalent contacts that Rutin creates improves its affinity. These interactions include five hydrogen bonds within the crucial ASN180–HIS218 residue cluster. Additionally, the stabilisation of hydrophobic and van der Waals contacts with PRO238, SER239, and TYR240 contributes to the formation of this network. The observation that flavonoid glycosides frequently exhibit increased binding and inhibitory potential towards metalloproteinases is well-established, and these binding qualities are in agreement with that observation. This is because flavonoid glycosides have a higher interaction surface area and extensive polar interactions. Priani et al. (2021) revealed that flavonoid glycosides exhibit substantial metalloproteinase inhibition due to cooperative binding interactions; these findings are in agreement with their findings.

In the collagenase active site, it is interesting to note that all of the ligands that were tested consistently engaged a group of conserved residues. These residues include ASN180, LEU181, ALA182, ARG214, and HIS218, respectively. In previous docking investigations of flavonoids and polyphenols against collagenase-like enzymes, it was observed that common active-site anchoring residues mediate binding across a variety of ligands. This constant engagement shows that these phenolic chemicals share a binding mechanism. This has also been observed in other docking studies.

Connections between the structure and function of phenolic enzyme inhibitors explain why binding energy changes. Caffeic and p-coumaric acids fit well into catalytic pockets. On the other hand, larger flavonoid glycosides like rutin use wider contact networks to make them more stable and more likely to stick to things. Furthermore, polyphenol studies indicate that hydrogen bonding and hydrophobic interactions enhance the inhibitory efficacy of tyrosinase and collagenase (Alkhadhrh et al., 2024; Mukattash, 2024). This docking study found that caffeic acid and rutin may inhibit tyrosinase and collagenase, respectively. These phytochemicals' binding characteristics and interaction networks follow broader patterns found in other natural phenolic and flavonoid compounds. Also, the role of phytochemicals in anti-aging and enzyme control is highlighted.

5.1 Study Limitations

Additionally, we solely do in vitro and in silico studies; in vivo and clinical trials are not planned at this time, although the findings may have dermatology and pharmacological uses.

Studying cardamom polyphenols' biological potential against S. aureus, collagenase, and tyrosinase will continue under controlled laboratory conditions. Beyond the current scope, safety profiling and formulation development should be researched.

There are a number of limitations that need to be addressed, despite the fact that the purpose of this work is to provide significant insights into the biological potential of polyphenols found in E. cardamomum:

- **In Vitro Nature of the Study**: Every experiment is done in a monitored lab. In addition, in vitro studies provide initial data but cannot replicate the complex environment of living beings. However, results cannot directly predict clinical outcomes or in vivo efficacy.
- **Single Bacterial Strain**: Only the common reference strain *S. aureus* (ATCC 25923) will be used to evaluate antibacterial activity. The results might not apply to other bacteria, such as Gram-negative species or resistant clinical isolates.
- **Limited Concentration Range**: Testing is done on the extract at a few different concentrations. Studies with an expanded concentration gradient may produce more thorough pharmacological profiles, even though dose-response associations will be studied.
- **Absence of Toxicological Assessment**: This stage of the study does not involve an assessment of cytotoxicity or skin safety. Therefore, even though biological activity may be shown, the extract's safety and acceptability for human use have not been evaluated.
- **Usage of other solvents:** Not all compounds can be extracted by the same solvents.

5.2 Conclusion

This research made a significant improvement to the scientific and pharmaceutical research area, by addressing a gap in the body of knowledge regarding *Elettaria cardamomum's* polyphenolic chemicals and their activities. As the essential oil extract of cardamom has been the focus of many previous researchers, nevertheless, its polyphenolic components and their inhibitory effects against microbial pathogens and important skin-related enzymes have received limited attention in the literature.

The ethanolic extract of *E. cardamomum*, contained natural plant compounds mainly polyphenols, which possess antibacterial, enzyme-inhibitory, and antioxidant properties. Where Molecular docking of these compounds showed that p-coumaric acid, and rutin against human tyrosinase and collagenase yielded stable binding poses. Molecular docking investigations further revealed the enzyme inhibitory properties of the identified phenolic compounds. In silico studies showed that some polyphenols exhibit stable and energetically favourable binding interactions with human collagenase and tyrosinase active sites. Caffeic acid strongly bound tyrosinase, while rutin bound collagenase. Our findings support the multifunctional potential of E. cardamomum extracts in cosmeceutical and pharmaceutical applications and suggest a molecular basis for the observed anti-aging and anti-hyperpigmentation benefits. By showing Elettaria cardamomum polyphenolic extracts' multi-target efficacy, this study advances science. Integrating phytochemical analysis, biological assessment, and computational modelling achieves this. The data suggest that this plant may be a source of bioactive compounds with antibacterial, antioxidant, anti-aging, and skin-lightening properties. This is promising, but further in vivo, toxicological, and clinical study is needed to establish the substance's efficacy and safety. this study provides a solid scientific foundation for future research and suggests that unique natural formulations developed from E. cardamomum may be exploited in the pharmaceutical and cosmeceutical industries.

5.3 Recommendation

Based on the current study, which showed that the ethanolic extract of Elettaria cardamomum contains polyphenolic compounds with antimicrobial, antioxidant, and enzyme inhibitory properties, the following recommendations have been made for future research and practical applications:

1. Recommendations for Future Research

1. Validation studies in vivo. Future research should evaluate the biological activities of E. cardamomum polyphenolic extracts in vivo using animal models. Such studies are necessary to confirm in vitro and in silico antimicrobial, antioxidant, anti-collagenase, and anti-tyrosinase effects and assess pharmacokinetics, bioavailability, and metabolic stability.
2. Toxicological and safety evaluation, to assess E. cardamomum extract and isolated phenolic compound safety, acute and chronic toxicity studies should be conducted. Keratinocytes and fibroblasts from normal human skin should be tested for cytotoxicity prior to clinical or industrial use.
3. Active compound isolation and characterisation. Further fractionation and purification of individual phenolic constituents is recommended to identify the biologically active compounds. To fully characterise isolated bioactive molecules, NMR and FTIR can be used.
4. Mechanical and molecular research. Further molecular-level research is needed to elucidate how polyphenols inhibit collagenase and tyrosinase. Enzyme kinetics and gene-expression analyses of oxidative stress and inflammation pathways would improve mechanistic understanding.
5. Enhanced antimicrobial range. To fully assess the antimicrobial potential of E. cardamomum extracts, future studies should test them against Gram-negative bacteria, fungi, and multidrug-resistant strains.

2. Recommendations for Pharmaceutical and Cosmeceutical Applications

1. Development of topical formulations. The findings support the potential incorporation of *E. cardamomum* polyphenolic extracts into topical dosage forms such as creams, gels, emulsions, and serums for antimicrobial, anti-aging, and skin-lightening applications.

2. Synthetic inhibitors versus natural. E. cardamomum extracts may be safer than synthetic collagenase and tyrosinase inhibitors due to their enzyme-inhibitory activity.Studies on formulation and stability. Further formulation studies should assess E. cardamomum extracts' physicochemical stability, shelf life, and controlled-release behaviour under different storage conditions.

3. Recommendations for Academic and Industrial Stakeholders

1. Collaborating across fields. Pharmacologists, microbiologists, cosmetic chemists, and formulation scientists should collaborate to commercialise lab findings.
2. Sustainable use of natural resources. For environmental responsibility and long-term raw material availability, researchers and manufacturers should source and grow E. cardamomum sustainably.

Elettaria cardamomum is a promising natural source of biomedical and cosmeceutical multifunctional polyphenolic compounds, according to this study. Experimental, computational, and clinical research are recommended to maximise therapeutic potential and develop safe, effective, and sustainable natural products.

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Appendices

Appendices (1) GC/MS Analysis

Sample Information

Analyzed by	: AAU
Analyzed	: 12/10/2025 11:24:03 AM
Sample Type	: Unknown
Level #	: 1
Sample Name	: PLANT EXTRACT
Sample ID	: 01
IS Amount	: [1]=1
Sample Amount	: 1
Dilution Factor	: 1
Vial #	: 1
Injection Volume	: 1.00
Data File	: C:\GCMSsolution\Data\EXTERNAL 10 12 2025\PLANT EXTRACTS 10 12 2025-001.qgd
Org Data File	: C:\GCMSsolution\Data\EXTERNAL 10 12 2025\PLANT EXTRACTS 10 12 2025-001.qgd
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Report File	: C:\GCMSsolution\Data\FORMAT 25 3 25.qgr
Tuning File	: C:\GCMSsolution\Data\20022025 TUNNING.qgt
Modified by	: AAU
Modified	: 12/10/2025 11:51:03 AM

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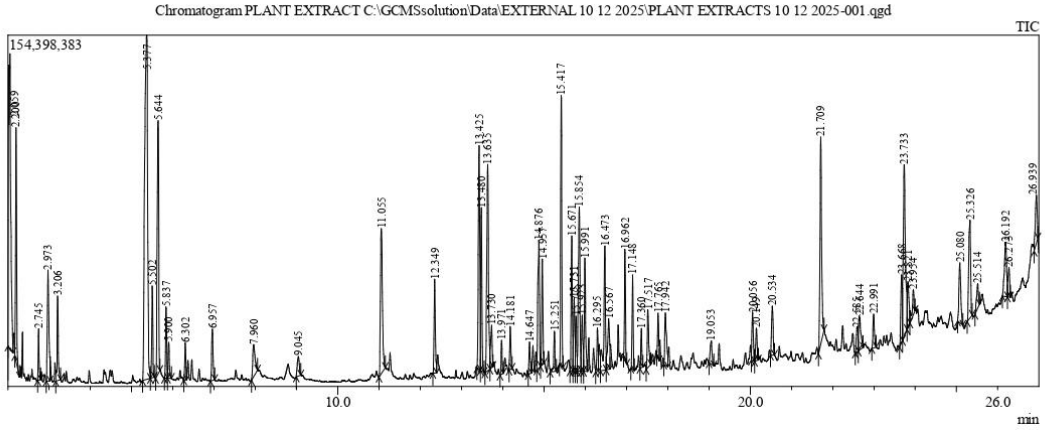

Peak Report TIC

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
1	2.059	2.005	2.125	466102689	7.22	102281976	4.30	4.56	E	1,3-Dioxolane, 4-methyl-2-(2-methylpropyl
2	2.200	2.165	2.285	177346022	2.75	102814709	4.32	1.72		Oxirane, 2,2'-(1,4-butanediyl)bis-
3	2.745	2.720	2.795	33619503	0.52	22559448	0.95	1.49		Tetrahydrofuran, 2,2-dimethyl-
4	2.973	2.930	3.020	129561214	2.01	48705437	2.05	2.66		3-Heptanol
5	3.206	3.160	3.280	72608530	1.12	37179530	1.56	1.95	V	3-Pentanol, 2,3-dimethyl-
6	5.377	5.265	5.455	720302218	11.15	130955004	5.50	5.50	E	2-Pentanone, 5-(acetyloxy)-
7	5.502	5.455	5.550	75814837	1.17	40327112	1.69	1.88	V	Pentanoic acid, 2-propenyl ester
8	5.644	5.585	5.685	289425419	4.48	111234174	4.67	2.60		2,5-Monomethylene-l-rhamnitol
9	5.837	5.795	5.870	58990046	0.91	31311856	1.32	1.88		1,2,6-Hexanetriol
10	5.900	5.870	5.965	32157734	0.50	15830362	0.67	2.03	V	Allyl isovalerate
11	6.302	6.265	6.335	29722517	0.46	16247360	0.68	1.83		Benzene, 1-ethyl-4-methyl-
12	6.957	6.910	7.015	53397930	0.83	22516022	0.95	2.37		Mesitylene
13	7.960	7.905	8.055	56622376	0.88	14081130	0.59	4.02		2,5-Dihydroxybenzaldehyde, 2TMS derivat
14	9.045	8.990	9.105	29309417	0.45	8565385	0.36	3.42		Cyclotetrasiloxane, octamethyl-
15	11.055	11.000	11.150	213445782	3.30	63730931	2.68	3.35		1,3,5-Benzetriol, 3TMS derivative
16	12.349	12.305	12.395	86538342	1.34	41250470	1.73	2.10		Cyclopentasiloxane, decamethyl-
17	13.425	13.375	13.455	244700753	3.79	98319788	4.13	2.49		.alpha.-Terpinyl acetate
18	13.480	13.455	13.550	144563088	2.24	71599182	3.01	2.02	V	Dodecanedioic acid, 2TBDMS derivative
19	13.635	13.570	13.690	265642805	4.11	90664831	3.81	2.93		1,3,5-Benzetriol, 3TMS derivative
20	13.730	13.690	13.765	47485067	0.74	18605869	0.78	2.55	V	Hexasiloxane, tetradecamethyl-
21	13.971	13.935	14.010	26424022	0.41	14811369	0.62	1.78		Cyclohexasiloxane, dodecamethyl-
22	14.181	14.150	14.225	34998008	0.54	18736716	0.79	1.87	V	Dodecanedioic acid, 2TBDMS derivative

Peak#	R.Time	I.Time	F.Time	Area	Area%	Height	Height%	A/H	Mark	Name
23	14.647	14.615	14.695	28836553	0.45	13857641	0.58	2.08		Cycloheptasiloxane, tetradecamethyl-
24	14.876	14.825	14.915	152844662	2.37	56156369	2.36	2.72	V	Cycloheptasiloxane, tetradecamethyl-
25	14.957	14.915	15.000	90171392	1.40	46484461	1.95	1.94	V	Cycloheptasiloxane, tetradecamethyl-
26	15.251	15.150	15.300	35355229	0.55	17591594	0.74	2.01	V	Cycloheptasiloxane, tetradecamethyl-
27	15.417	15.370	15.465	223878961	3.47	118718343	4.99	1.89		Cyclononasiloxane, octadecamethyl-
28	15.671	15.630	15.705	119825782	1.85	59276649	2.49	2.02		Dodecanedioic acid, 2TBDMS derivative
29	15.731	15.705	15.755	66710536	1.03	32068390	1.35	2.08	V	Dodecanedioic acid, 2TBDMS derivative
30	15.775	15.755	15.805	46058166	0.71	24060524	1.01	1.91	V	Dodecanedioic acid, 2TBDMS derivative
31	15.854	15.805	15.895	192394126	2.98	72129562	3.03	2.67	V	Cyclooctasiloxane, hexadecamethyl-
32	15.923	15.895	15.960	58205645	0.90	24632957	1.03	2.36	V	Cyclooctasiloxane, hexadecamethyl-
33	15.991	15.960	16.055	111479301	1.73	49794425	2.09	2.24	V	Heptasiloxane, hexadecamethyl-
34	16.295	16.250	16.320	39834946	0.62	19086977	0.80	2.09	V	Citric acid, 4TBDMS derivative
35	16.473	16.365	16.510	149160290	2.31	54601160	2.29	2.73	V	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-,
36	16.567	16.510	16.600	72164539	1.12	22266428	0.94	3.24	V	8-Hydroxycarvotanacetone
37	16.962	16.930	17.005	79321972	1.23	48261584	2.03	1.64		Cyclooctasiloxane, hexadecamethyl-
38	17.148	17.105	17.190	74777995	1.16	41498466	1.74	1.80		Cyclooctasiloxane, hexadecamethyl-
39	17.360	17.325	17.395	29994061	0.46	17251341	0.72	1.74		Cycloheptasiloxane, tetradecamethyl-
40	17.517	17.480	17.585	61786117	0.96	25444548	1.07	2.43		Cycloheptasiloxane, tetradecamethyl-
41	17.765	17.735	17.795	38944227	0.60	19406303	0.82	2.01		Cyclooctasiloxane, hexadecamethyl-
42	17.942	17.905	18.000	69065951	1.07	22912153	0.96	3.01		Cyclooctasiloxane, hexadecamethyl-
43	19.053	19.000	19.115	31287159	0.48	10190206	0.43	3.07		Cyclononasiloxane, octadecamethyl-
44	20.056	20.025	20.100	47909184	0.74	21098649	0.89	2.27	V	1-Naphthalenepropanol, .alpha.-ethenyldeca
45	20.149	20.105	20.195	31761675	0.49	14229806	0.60	2.23		Pentadecanal-
46	20.534	20.490	20.590	55879069	0.86	21509846	0.90	2.60		1,2-Benzenedicarboxylic acid, bis(2-methyl
47	21.709	21.655	21.790	250120350	3.87	91086404	3.83	2.75		n-Hexadecanoic acid
48	22.585	22.545	22.620	34636650	0.54	10419781	0.44	3.32		Tetracosane
49	22.644	22.620	22.735	54272711	0.84	14998761	0.63	3.62	V	Tetracontane
50	22.991	22.950	23.050	35606107	0.55	14844158	0.62	2.40		Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7
51	23.668	23.620	23.690	75608431	1.17	29666431	1.25	2.55		9,12-Octadecadienoic acid (Z,Z)-
52	23.733	23.690	23.800	276668821	4.28	75407383	3.17	3.67	V	9-Octadecenoic acid, (E)-
53	23.821	23.800	23.870	58232484	0.90	20141897	0.85	2.89	V	Dihydrotachysterol
54	23.954	23.870	23.995	32904633	0.51	10986788	0.46	2.99	V	Octadecanoic acid
55	25.080	25.025	25.155	81752092	1.27	26405936	1.11	3.10		Dotriacontane
56	25.326	25.260	25.380	137926632	2.14	43048174	1.81	3.20		Pentatriacontane
57	25.514	25.450	25.560	34084118	0.53	10791842	0.45	3.16		Cyclononasiloxane, octadecamethyl-
58	26.192	26.115	26.235	89970972	1.39	23803962	1.00	3.78		1-Naphthalenepropanol, .alpha.-ethenyldeca
59	26.273	26.235	26.310	34530658	0.53	12904748	0.54	2.68	V	Tetracosane
60	26.939	26.880	26.975	67303274	1.04	20961875	0.88	3.21	V	Octadecane, 3-ethyl-5-(2-ethylbutyl)-
				6460043790	100.00	2380325183	100.00			

Library

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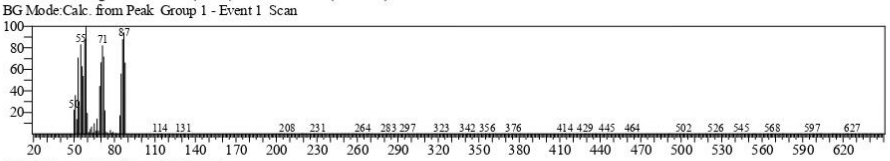

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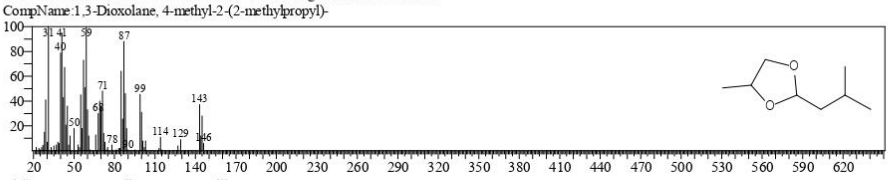

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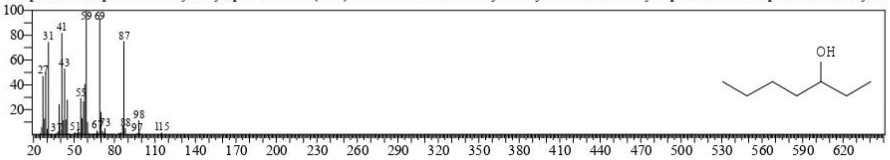

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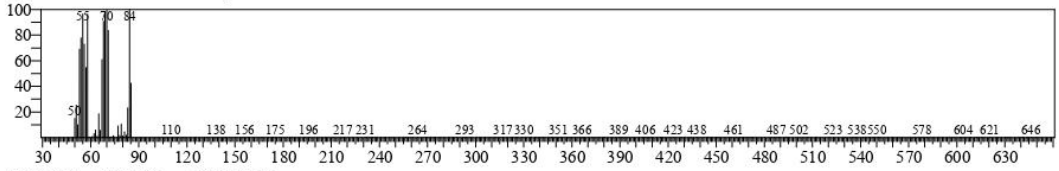

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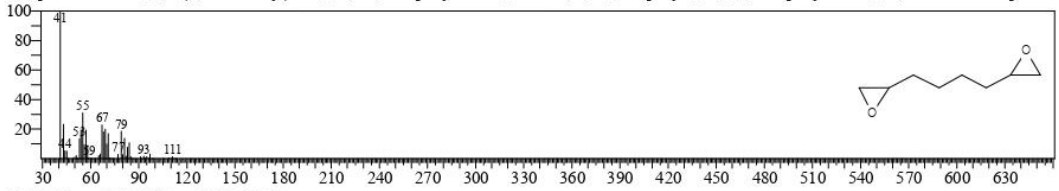

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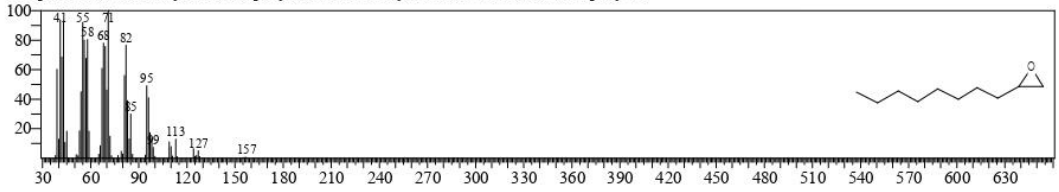

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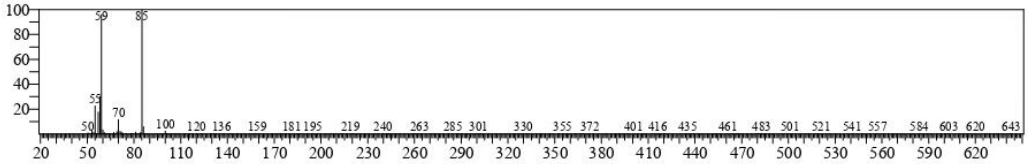

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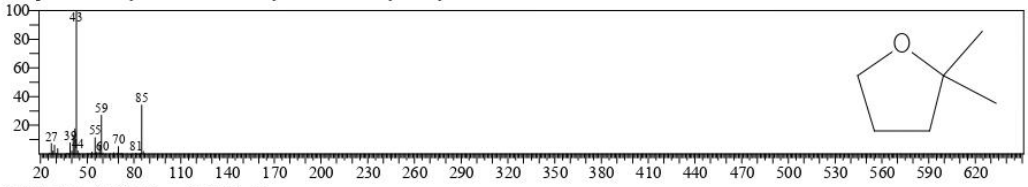
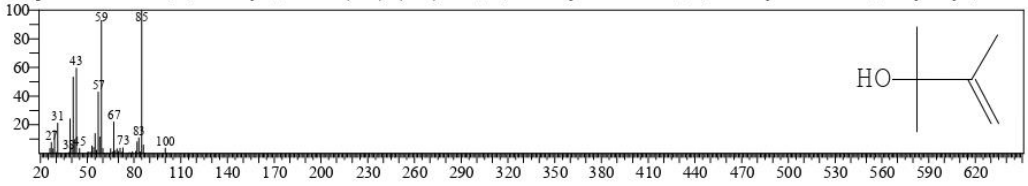
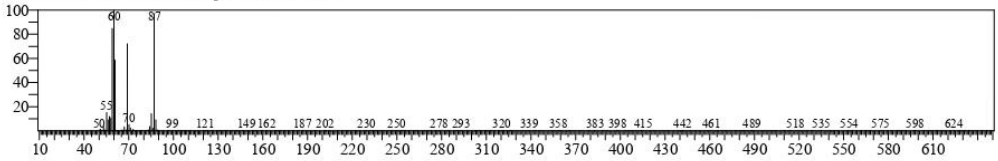
SI:93 Formula:C6H12O CAS:1003-17-4 MolWeight:100 RetIndex:723
CompName:Tetrahydrofuran, 2,2-dimethyl- $$ 2,2-Dimethyltetrahydrofuran $$



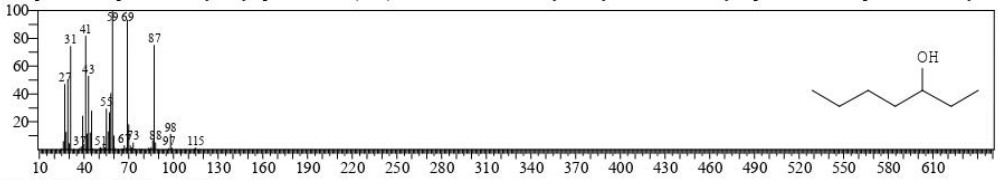
Hit#:2 Entry:2238 Library:NIST17s.lib
SI:89 Formula:C6H12O CAS:10473-13-9 MolWeight:100 RetIndex:677
CompName:3-Buten-2-ol, 2,3-dimethyl- $$ CH2=C(CH3)C(CH3)2OH $$ 2,3-Dimethyl-3-buten-2-ol $$ 2,3-Dimethyl-1-buten-3-ol $$ 3-Hydroxy-2,3-dime



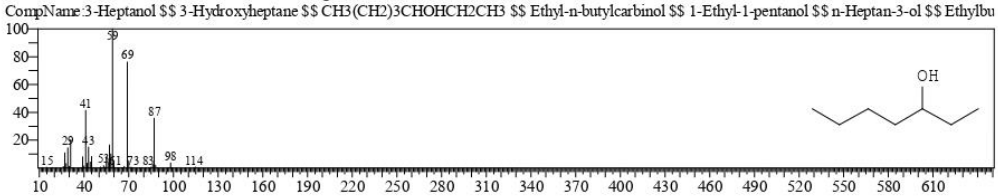
<< Target >>
Line#:4 R.Time:2.975(Scan#:196) MassPeaks:305
RawMode:Averaged 2.970-2.980(195-197) BasePeak:59.95(8273144)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



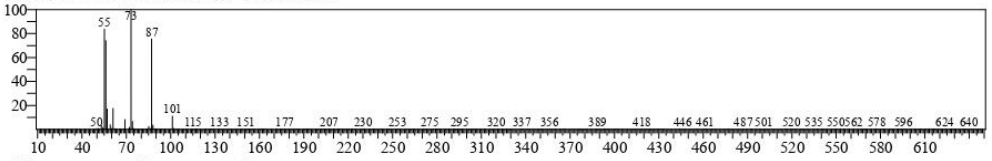
Hit#:1 Entry:4406 Library:NIST17s.lib
SI:82 Formula:C7H16O CAS:589-82-2 MolWeight:116 RetIndex:879
CompName:3-Heptanol $$ 3-Hydroxyheptane $$ CH3(CH2)3CHOHCH2CH3 $$ Ethyl-n-butylcarbinol $$ 1-Ethyl-1-pentanol $$ n-Heptan-3-ol $$ Ethylbu



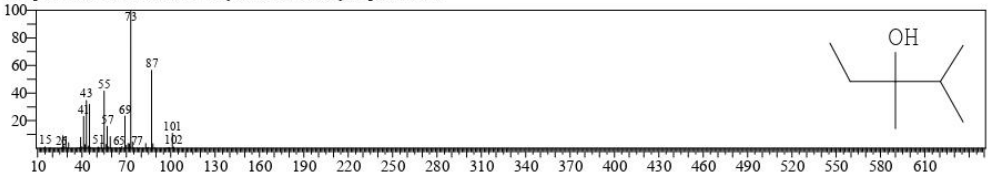
Hit#:2 Entry:4407 Library:NIST17s.lib
SI:81 Formula:C7H16O CAS:589-82-2 MolWeight:116 RetIndex:879
CompName:3-Heptanol $$ 3-Hydroxyheptane $$ CH3(CH2)3CHOHCH2CH3 $$ Ethyl-n-butylcarbinol $$ 1-Ethyl-1-pentanol $$ n-Heptan-3-ol $$ Ethylbu



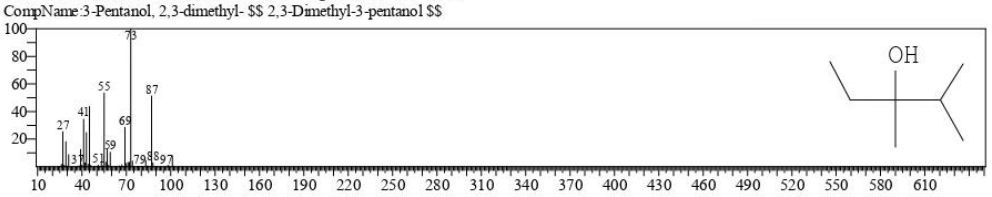
<< Target >>
Line#:5 R.Time:3.205(Scan#:242) MassPeaks:322
RawMode:Averaged 3.200-3.210(241-243) BasePeak:73.05(7840235)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



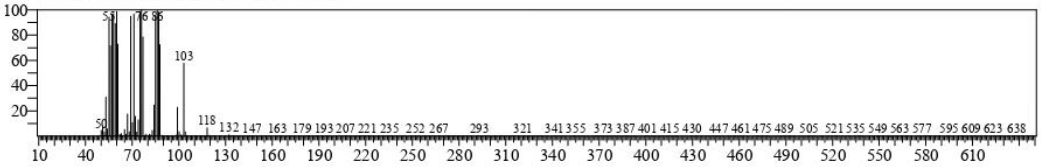
Hit#:1 Entry:4419 Library:NIST17s.lib
SI:84 Formula:C7H16O CAS:595-41-5 MolWeight:116 RetIndex:745
CompName:3-Pentanol, 2,3-dimethyl- $$ 2,3-Dimethyl-3-pentanol $$



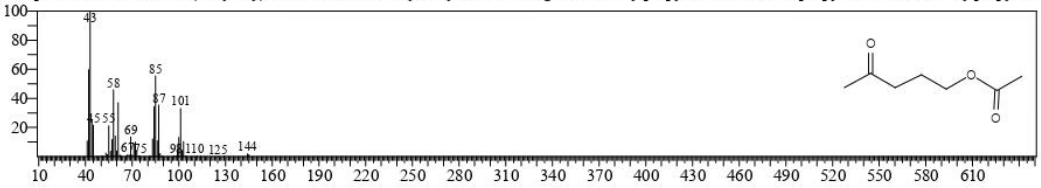
Hit#:2 Entry:4418 Library:NIST17s.lib
SI:84 Formula:C7H16O CAS:595-41-5 MolWeight:116 RetIndex:745
CompName:3-Pentanol, 2,3-dimethyl- $$ 2,3-Dimethyl-3-pentanol $$



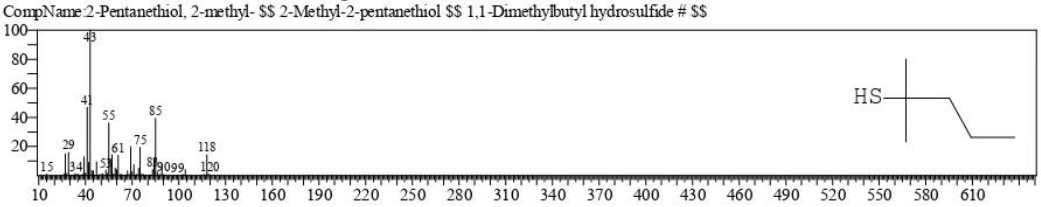
<< Target >>
Line#:6 R.Time:5.375(Scan#:676) MassPeaks:498
RawMode:Averaged 5.370-5.380(675-677) BasePeak:75.90(8371864)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



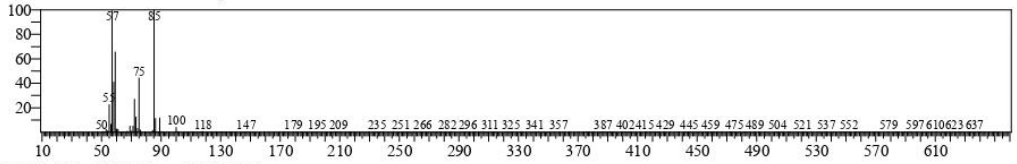
Hit#:1 Entry:9408 Library:NIST17s.lib
SI:69 Formula:C7H12O3 CAS:5185-97-7 MolWeight:144 RetIndex:1020
CompName:2-Pentanone, 5-(acetyloxy)- $$ 2-Pentanone, 5-hydroxy-, acetate $$ .gamma.-Acetylpropyl acetate $$ Acetopropyl acetate $$ 3-Acetylpropyl ac



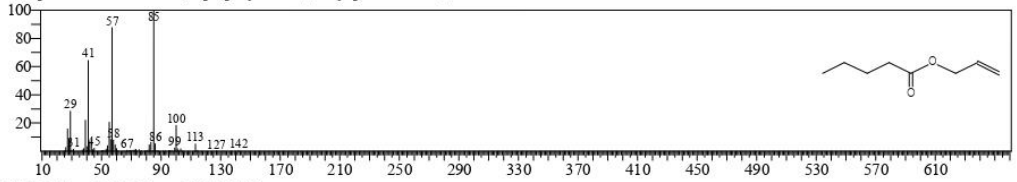
Hit#:2 Entry:4643 Library:NIST17s.lib
SI:69 Formula:C6H14S CAS:1633-97-2 MolWeight:118 RetIndex:837
CompName:2-Pentanethiol, 2-methyl- $$ 2-Methyl-2-pentanethiol $$ 1,1-Dimethylbutyl hydrosulfide # $$



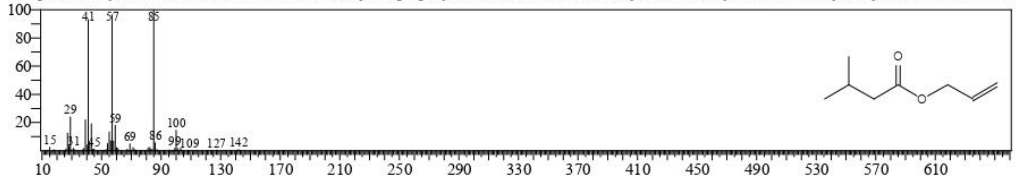
<< Target >>
Line#:7 R.Time:5.500(Scan#:701) MassPeaks:384
RawMode:Averaged 5.495-5.505(700-702) BasePeak:85.15(7833573)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



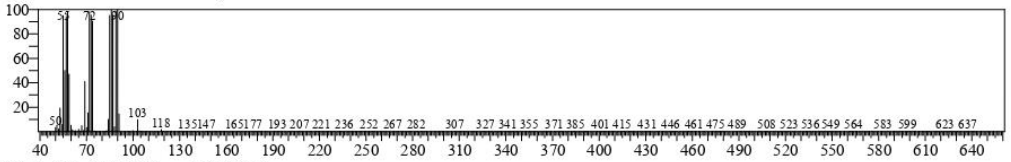
Hit#:1 Entry:9105 Library:NIST17s.lib
SI:80 Formula:C8H14O2 CAS:6321-45-5 MolWeight:142 RetIndex:974
CompName:Pentanoic acid, 2-propenyl ester $$ Allyl pentanoate # $$



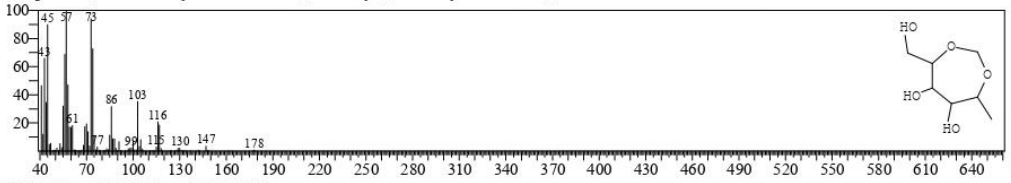
Hit#:2 Entry:9108 Library:NIST17s.lib
SI:80 Formula:C8H14O2 CAS:2835-39-4 MolWeight:142 RetIndex:910
CompName:Allyl isovalerate $$ Butanoic acid, 3-methyl-, 2-propenyl ester $$ Isovaleric acid, allyl ester $$ Butyric acid, 3-methyl-, allyl ester $$ NCI-C547



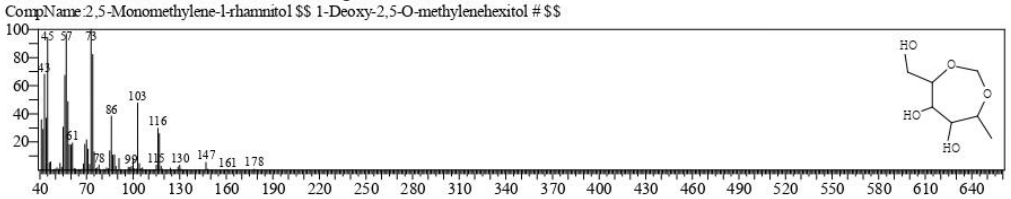
<< Target >>
Line#:8 R.Time:5.645(Scan#:730) MassPeaks:423
RawMode:Averaged 5.640-5.650(729-731) BasePeak:90.00(8351490)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



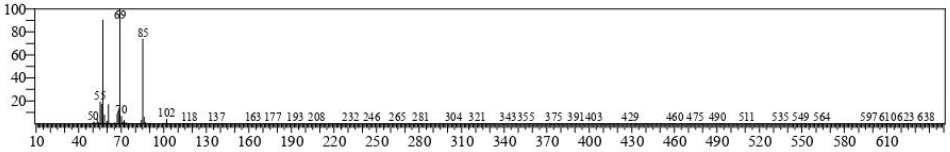
Hit#:1 Entry:16916 Library:NIST17s.lib
SI:72 Formula:C7H14O5 CAS:5399-33-7 MolWeight:178 RetIndex:1558
CompName:2,5-Monomethylene-l-rhamnitol $$ 1-Deoxy-2,5-O-methylenehexitol # $$



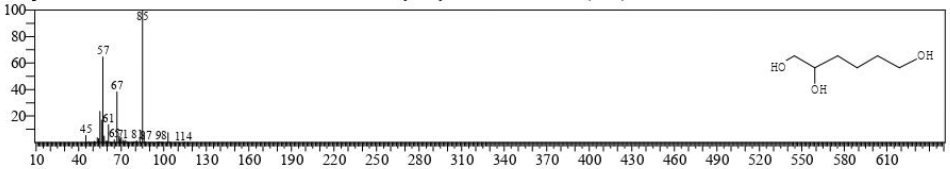
Hit#:2 Entry:16919 Library:NIST17s.lib
SI:72 Formula:C7H14O5 CAS:5399-33-7 MolWeight:178 RetIndex:1558
CompName:2,5-Monomethylene-l-rhamnitol $$ 1-Deoxy-2,5-O-methylenehexitol # $$



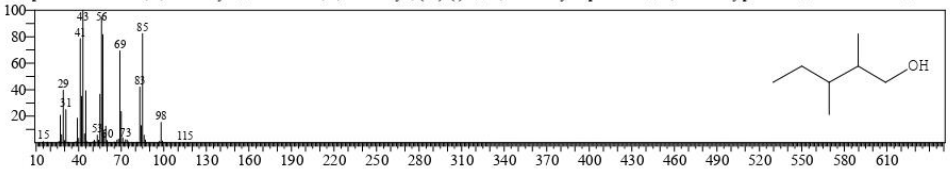
<< Target >>
Line#:9 R.Time:5.835(Scan#:768) MassPeaks:343
RawMode:Averaged 5.830-5.840(767-769) BasePeak:69.05(7320165)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



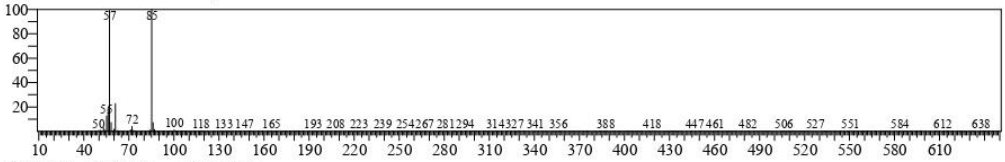
Hit#:1 Entry:7272 Library:NIST17s.lib
SI:83 Formula:C6H14O3 CAS:106-69-4 MolWeight:134 RetIndex:1265
CompName:1,2,6-Hexanetriol $$ Hexane-1,2,6-triol $$ 1,2,6-Trihydroxyhexane $$ Hexanetriol-(1,2,6) $$



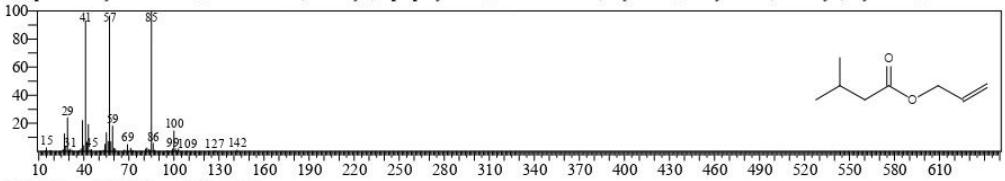
Hit#:2 Entry:4371 Library:NIST17s.lib
SI:81 Formula:C7H16O CAS:10143-23-4 MolWeight:116 RetIndex:832
CompName:1-Pentanol, 2,3-dimethyl- $$ 1-Pentanol, 2,3-dimethyl-, (3S)-(-)- $$ 2,3-Dimethyl-1-pentanol $$ 2,3-Dimethylpentanol $$ NSC 103151 $$



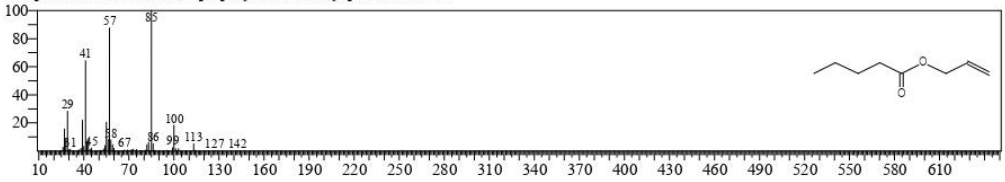
<< Target >>
Line#:10 R.Time:5.900(Scan#:781) MassPeaks:341
RawMode:Averaged 5.895-5.905(780-782) BasePeak:85.10(4651181)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



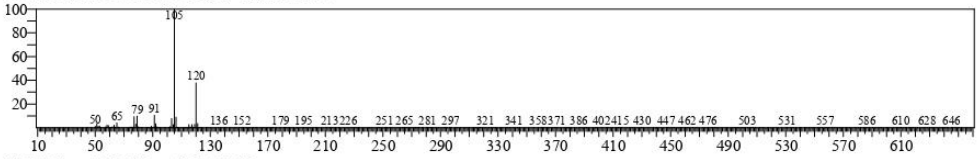
Hit#:1 Entry:9108 Library:NIST17s.lib
SI:90 Formula:C8H14O2 CAS:2835-39-4 MolWeight:142 RetIndex:910
CompName:Allyl isovalerate $$ Butanoic acid, 3-methyl-, 2-propenyl ester $$ Isovaleric acid, allyl ester $$ Butyric acid, 3-methyl-, allyl ester $$ NCI-C547



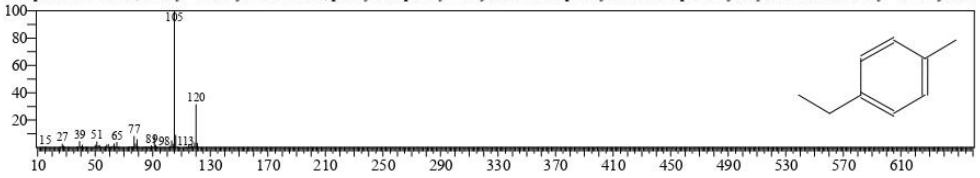
Hit#:2 Entry:9105 Library:NIST17s.lib
SI:88 Formula:C8H14O2 CAS:6321-45-5 MolWeight:142 RetIndex:974
CompName:Pentanoic acid, 2-propenyl ester $$ Allyl pentanoate # $$



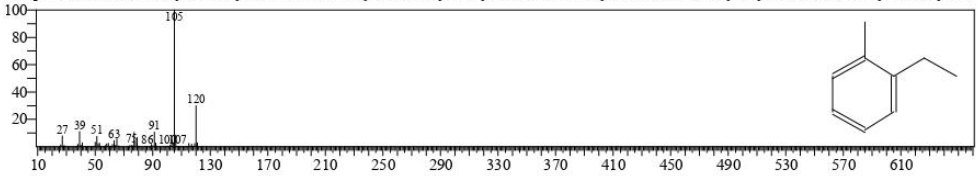
<< Target >>
Line#:11 R.Time:6.300(Scan#:861) MassPeaks:309
RawMode:Averaged 6.295-6.305(860-862) BasePeak:105.05(6487014)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



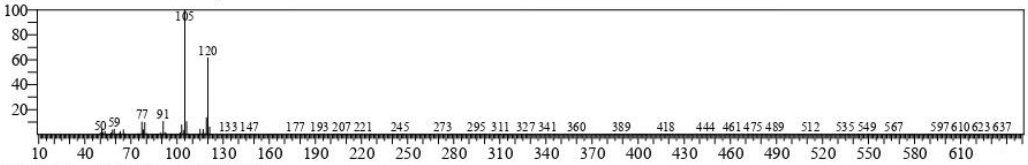
Hit#:1 Entry:4909 Library:NIST17s.lib
SI:97 Formula:C9H12 CAS:622-96-8 MolWeight:120 RetIndex:1006
CompName:Benzene, 1-ethyl-4-methyl- $$ Toluene, p-ethyl- $$ p-Ethylmethylbenzene $$ p-Ethyltoluene $$ p-Methylethylbenzene $$ 1-Ethyl-4-methylbenz



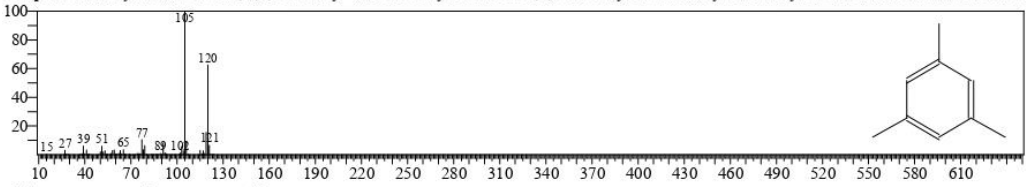
Hit#:2 Entry:4897 Library:NIST17s.lib
SI:96 Formula:C9H12 CAS:611-14-3 MolWeight:120 RetIndex:1006
CompName:Benzene, 1-ethyl-2-methyl- $$ Toluene, o-ethyl- $$ o-Ethylmethylbenzene $$ o-Ethyltoluene $$ o-Methylethylbenzene $$ 1-Ethyl-2-methylbenz



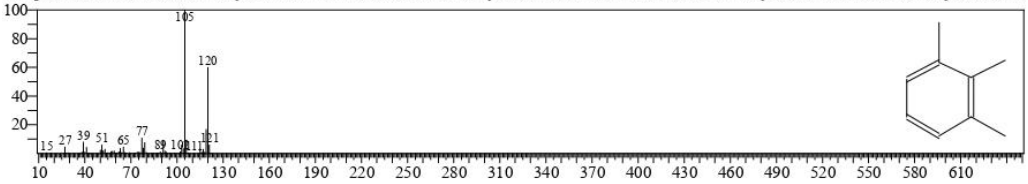
<< Target >>
Line#:12 R.Time:6.955(Scan#:992) MassPeaks:354
RawMode:Averaged 6.950-6.960(991-993) BasePeak:105.05(7743521)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



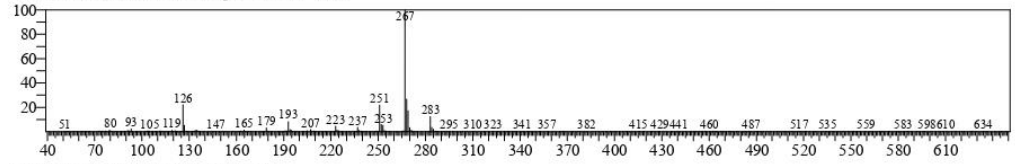
Hit#:1 Entry:4911 Library:NIST17s.lib
SI:97 Formula:C9H12 CAS:108-67-8 MolWeight:120 RetIndex:1020
CompName:Mesitylene $$ Benzene, 1,3,5-trimethyl- $$ s-Trimethylbenzene $$ 1,3,5-Trimethylbenzene $$ sym-Trimethylbenzene $$ Fleet-X $$ TMB $$ U



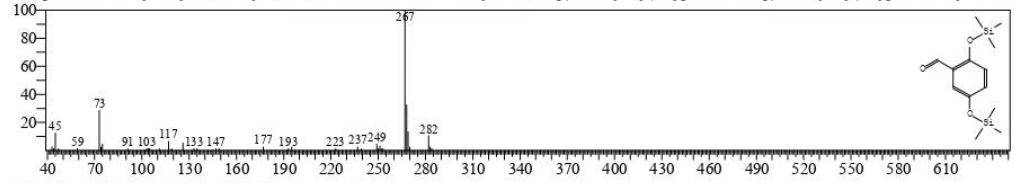
Hit#:2 Entry:4913 Library:NIST17s.lib
SI:97 Formula:C9H12 CAS:526-73-8 MolWeight:120 RetIndex:1020
CompName:Benzene, 1,2,3-trimethyl- $$ Hemimellitene $$ 1,2,3-Trimethylbenzene $$ Hemellitol $$ 1,2,3-Trimethyl benzene $$ 1,2,3-TrimethyIbenzene $



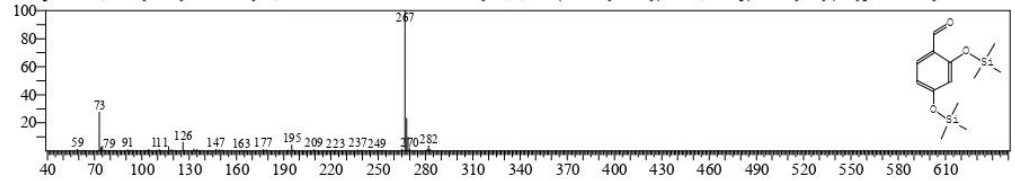
<< Target >>
Line#:13 R.Time:7.960(Scan#:1193) MassPeaks:387
RawMode:Averaged 7.955-7.965(1192-1194) BasePeak:267.00(4943547)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



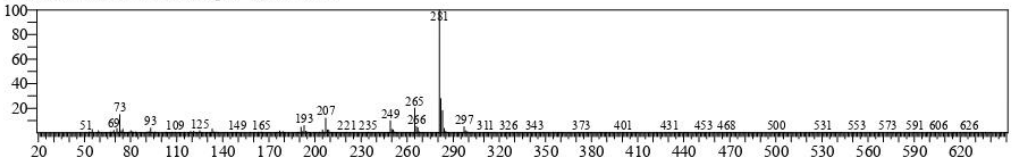
Hit#:1 Entry:31564 Library:NIST17s.lib
SI:79 Formula:C13H22O3Si2 CAS:56114-69-3 MolWeight:282 RetIndex:1578
CompName:2,5-Dihydroxybenzaldehyde, 2TMS derivative $$ Benzaldehyde, 2,5-bis[(trimethylsilyl)oxy]- $$ 2,5-Bis[(trimethylsilyl)oxy]benzaldehyde # $$



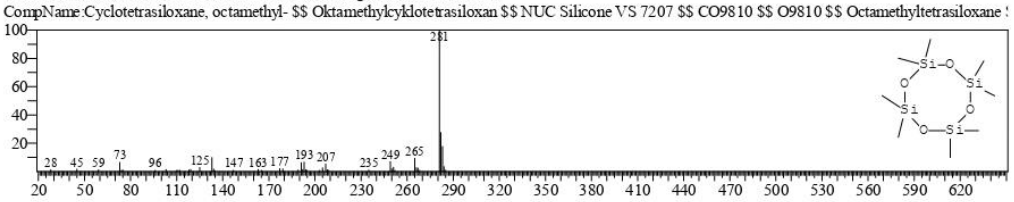
Hit#:2 Entry:31563 Library:NIST17s.lib
SI:79 Formula:C13H22O3Si2 CAS:33617-38-8 MolWeight:282 RetIndex:1578
CompName:2,4-Dihydroxybenzaldehyde, 2TMS derivative $$ Benzaldehyde, 2,4-bis(trimethylsiloxy)- $$ 2,4-Bis[(trimethylsilyl)oxy]benzaldehyde # $$



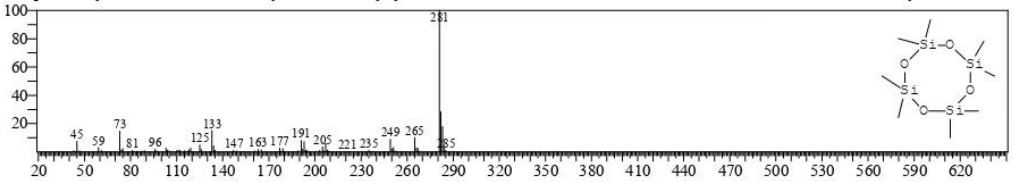
<< Target >>
Line#:14 R.Time:9.045(Scan#:1410) MassPeaks:372
RawMode:Averaged 9.040-9.050(1409-1411) BasePeak:281.05(2799358)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



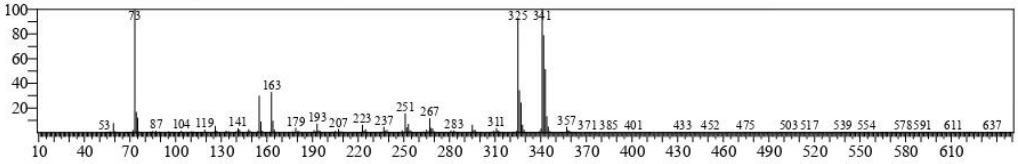
Hit#:1 Entry:32686 Library:NIST17s.lib
SI:88 Formula:C8H24O4Si4 CAS:556-67-2 MolWeight:296 RetIndex:827
CompName:Cyclotetrasiloxane, octamethyl- $$ Oktamethylcyklotetrasiloxan $$ NUC Silicone VS 7207 $$ CO9810 $$ O9810 $$ Octamethyltetrasiloxane



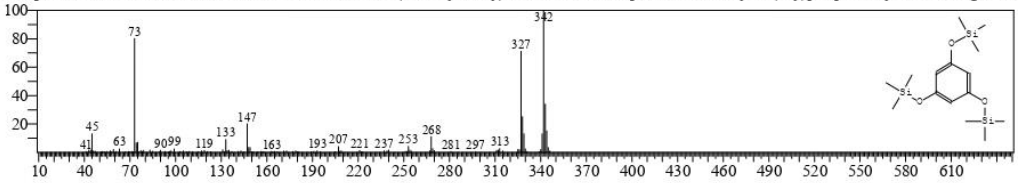
Hit#:2 Entry:32687 Library:NIST17s.lib
SI:87 Formula:C8H24O4Si4 CAS:556-67-2 MolWeight:296 RetIndex:827
CompName:Cyclotetrasiloxane, octamethyl- $$ Oktamethylcyklotetrasiloxan $$ NUC Silicone VS 7207 $$ CO9810 $$ O9810 $$ Octamethyltetrasiloxane



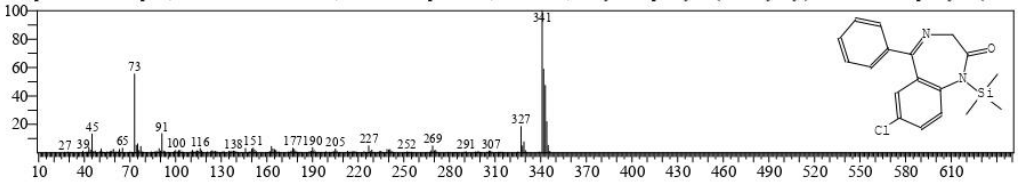
<< Target >>
Line#:15 R.Time:11.055(Scan#:1812) MassPeaks:437
RawMode:Averaged 11.050-11.060(1811-1813) BasePeak:341.05(7836428)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



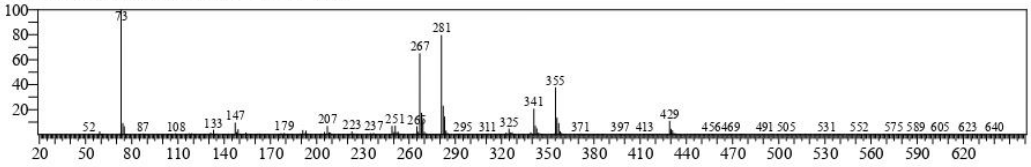
Hit#:1 Entry:35576 Library:NIST17s.lib
SI:65 Formula:C15H30O3Si3 CAS:10586-12-6 MolWeight:342 RetIndex:1574
CompName:1,3,5-Benzetriol, 3TMS derivative $$ 1,3,5-Tris(trimethylsiloxy)benzene $$ Silane, [1,3,5-benzenetriyltris(oxy)]tris[trimethyl- $$ Phloroglucinc



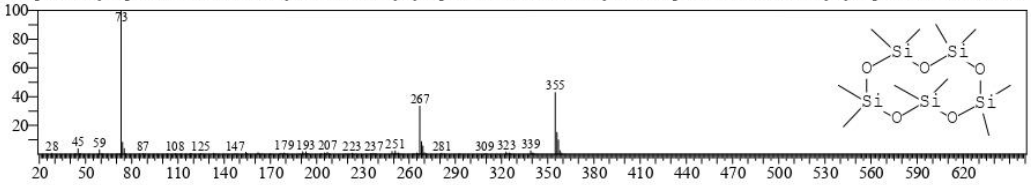
Hit#:2 Entry:35586 Library:NIST17s.lib
SI:63 Formula:C18H19ClN2OSi CAS:55299-24-6 MolWeight:342 RetIndex:2579
CompName:Nordazepam, TMS derivative $$ 2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-1-(trimethylsilyl)- $$ 7-Chloro-5-phenyl-1-(trim



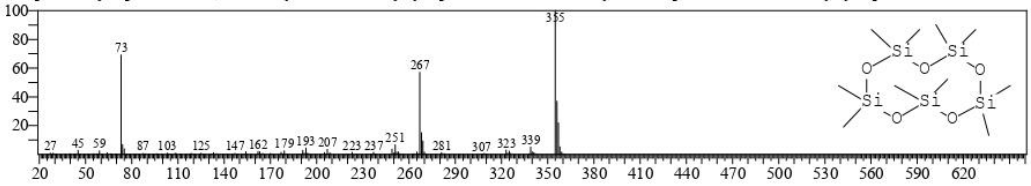
<< Target >>
Line#:16 R.Time:12.350(Scan#:2071) MassPeaks:412
RawMode:Averaged 12.345-12.355(2070-2072) BasePeak:73.00(6808738)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



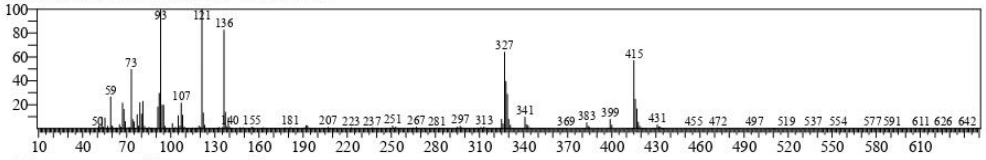
Hit#:1 Entry:36727 Library:NIST17s.lib
SI:75 Formula:C10H30O5Si5 CAS:541-02-6 MolWeight:370 RetIndex:1034
CompName:Cyclopentasiloxane, decamethyl- $$ Decamethylcyclopentasiloxane $$ Dimethylsiloxane pentamer $$ Dekamethylcyklopentasiloxan $$ CD377



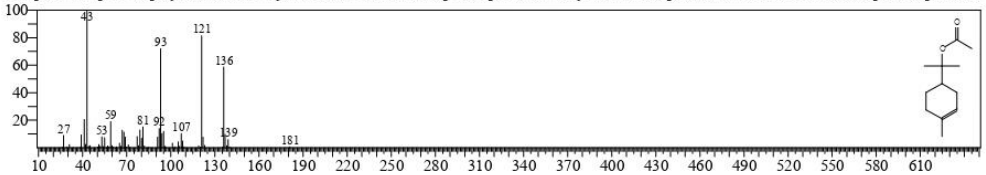
Hit#:2 Entry:36728 Library:NIST17s.lib
SI:73 Formula:C10H30O5Si5 CAS:541-02-6 MolWeight:370 RetIndex:1034
CompName:Cyclopentasiloxane, decamethyl- $$ Decamethylcyclopentasiloxane $$ Dimethylsiloxane pentamer $$ Dekamethylcyklopentasiloxan $$ CD377



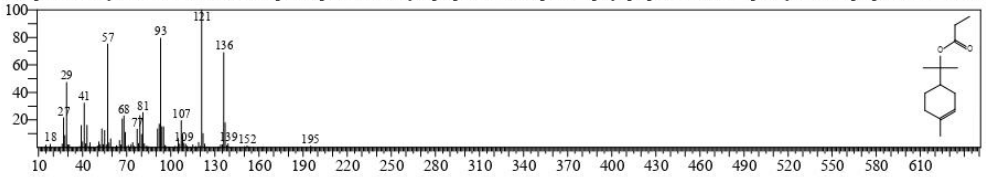
<< Target >>
Line#:17 R.Time:13.425(Scan#:2286) MassPeaks:412
RawMode:Averaged 13.420-13.430(2285-2287) BasePeak:121.15(7470835)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



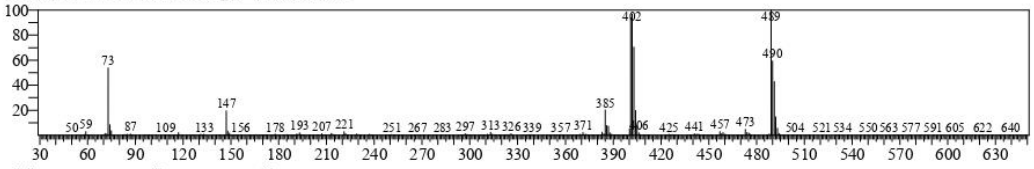
Hit#:1 Entry:20785 Library:NIST17s.lib
SI:71 Formula:C12H20O2 CAS:80-26-2 MolWeight:196 RetIndex:1333
CompName:.alpha.-Terpinyl acetate $$ 3-Cyclohexene-1-methanol, .alpha., alpha.,4-trimethyl-, acetate $$ p-Menth-1-en-8-ol, acetate $$ .alpha.-Terpineol ac



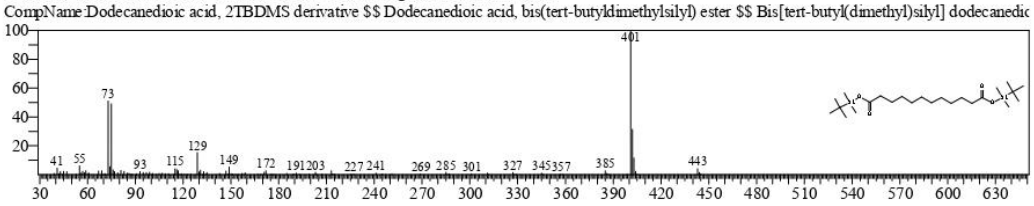
Hit#:2 Entry:23427 Library:NIST17s.lib
SI:69 Formula:C13H22O2 CAS:80-27-3 MolWeight:210 RetIndex:1432
CompName:3-Cyclohexene-1-methanol, .alpha., alpha.,4-trimethyl-, propanoate $$ .alpha.-Terpinyl propionate $$ 4-Terpinenyl ester of propanoic acid $$ .al



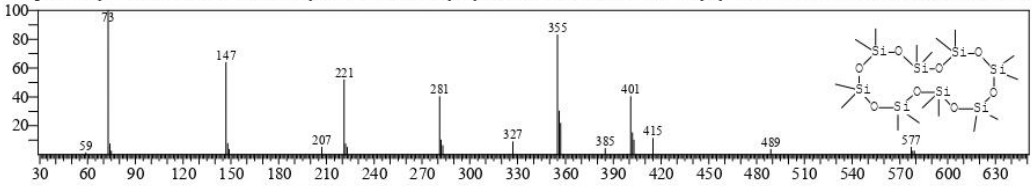
<< Target >>
Line#:18 R.Time:13.480(Scan#:2297) MassPeaks:402
RawMode:Averaged 13.475-13.485(2296-2298) BasePeak:489.05(7060113)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



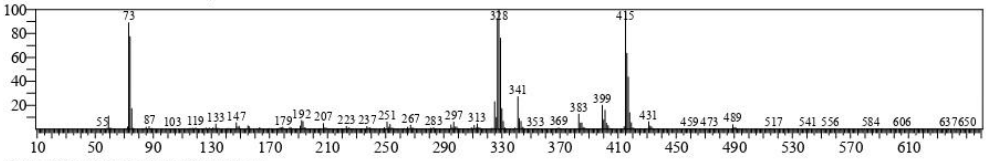
Hit#:1 Entry:38461 Library:NIST17s.lib
SI:53 Formula:C24H50O4Si2 CAS:104255-99-4 MolWeight:458 RetIndex:2392
CompName:Dodecanedioic acid, 2TBDMS derivative $$ Dodecanedioic acid, bis(tert-butyldimethylsilyl) ester $$ Bis[tert-butyl(dimethyl)silyl] dodecanedic



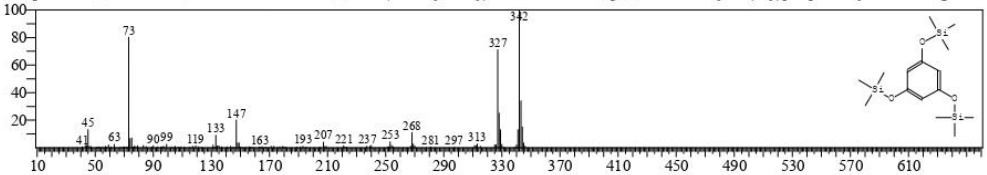
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:46 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



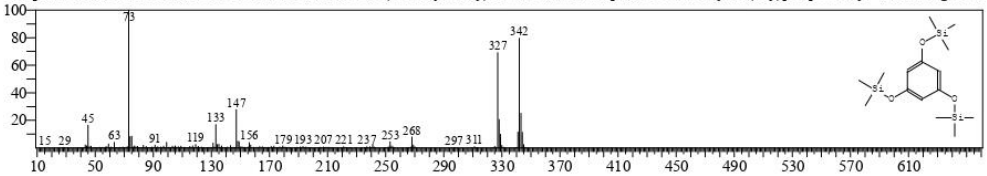
<< Target >>
Line#:19 R.Time:13.635(Scan#:2328) MassPeaks:472
RawMode:Averaged 13.630-13.640(2327-2329) BasePeak:327.85(8036878)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



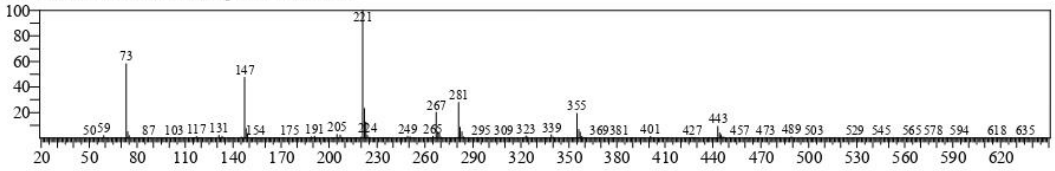
Hit#:1 Entry:35576 Library:NIST17s.lib
SI:54 Formula:C15H30O3Si3 CAS:10586-12-6 MolWeight:342 RetIndex:1574
CompName:1,3,5-Benzetriol, 3TMS derivative $$ 1,3,5-Tris(trimethylsiloxy)benzene $$ Silane, [1,3,5-benzenetriyltris(oxy)]tris[trimethyl- $$ Phloroglucinc



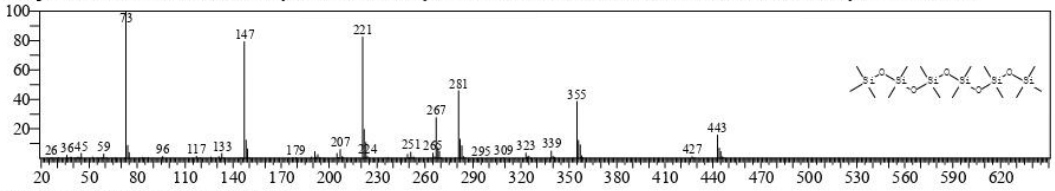
Hit#:2 Entry:35575 Library:NIST17s.lib
SI:51 Formula:C15H30O3Si3 CAS:10586-12-6 MolWeight:342 RetIndex:1574
CompName:1,3,5-Benzetriol, 3TMS derivative $$ 1,3,5-Tris(trimethylsiloxy)benzene $$ Silane, [1,3,5-benzenetriyltris(oxy)]tris[trimethyl- $$ Phloroglucinc



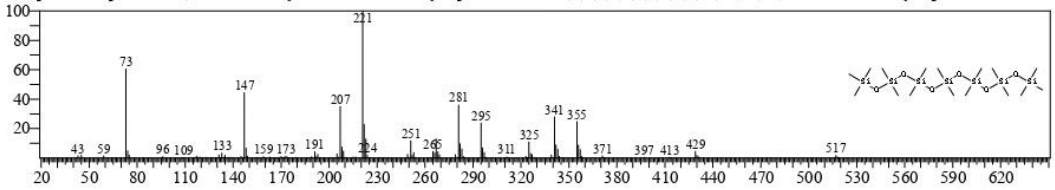
<< Target >>
Line#:20 R.Time:13.730(Scan#:2347) MassPeaks:315
RawMode:Averaged 13.725-13.735(2346-2348) BasePeak:221.05(3685716)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



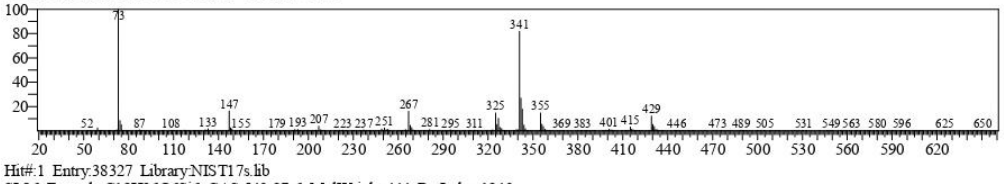
Hit#:1 Entry:38451 Library:NIST17s.lib
SI:88 Formula:C14H42O5Si6 CAS:107-52-8 MolWeight:458 RetIndex:1252
CompName:Hexasiloxane, tetradecamethyl- $$ Tetradecamethylhexasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,11-Tetradecamethylhexasiloxane # $$



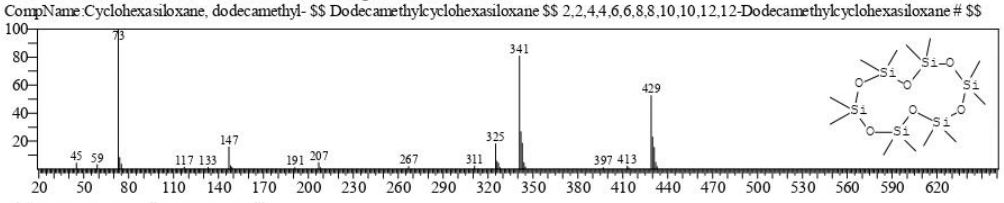
Hit#:2 Entry:38891 Library:NIST17s.lib
SI:79 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane # $$



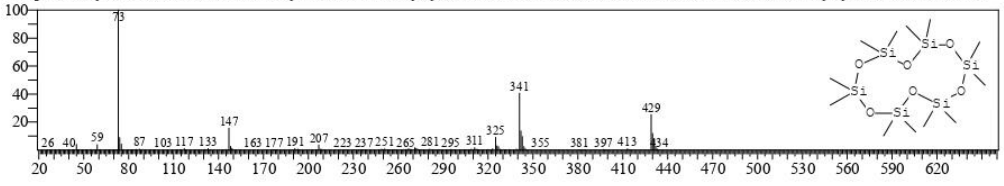
<< Target >>
Line#:21 R.Time:13.970(Scan#:2395) MassPeaks:416
RawMode:Averaged 13.965-13.975(2394-2396) BasePeak:73.05(3314226)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



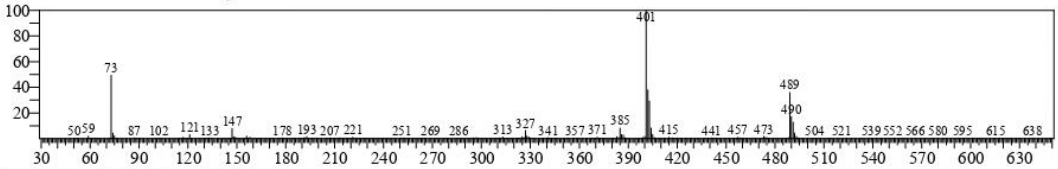
Hit#:1 Entry:38327 Library:NIST17s.lib
SI:86 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:1240
CompName:Cyclohexasiloxane, dodecamethyl- $$ Dodecamethylcyclohexasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12-Dodecamethylcyclohexasiloxane # $$



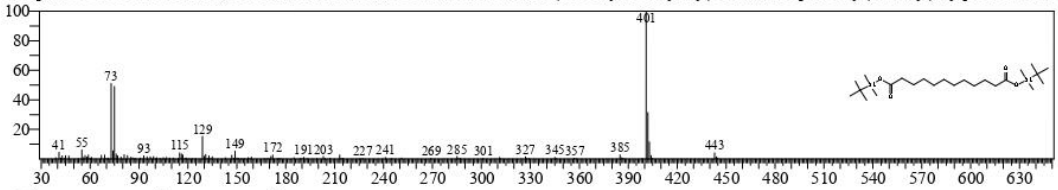
Hit#:2 Entry:38328 Library:NIST17s.lib
SI:83 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:1240
CompName:Cyclohexasiloxane, dodecamethyl- $$ Dodecamethylcyclohexasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12-Dodecamethylcyclohexasiloxane # $$



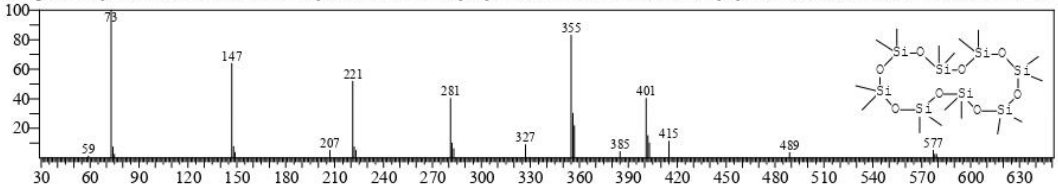
<< Target >>
Line#:22 R.Time:14.180(Scan#:2437) MassPeaks:386
RawMode:Averaged 14.175-14.185(2436-2438) BasePeak:401.00(4685743)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



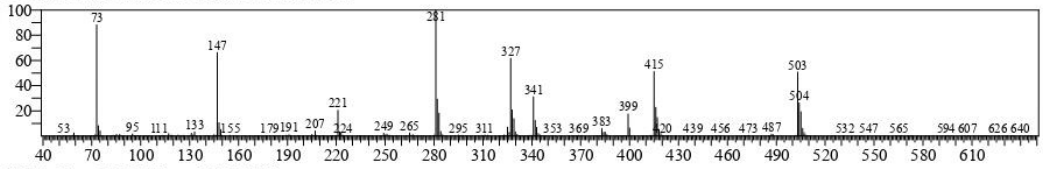
Hit#:1 Entry:38461 Library:NIST17s.lib
SI:67 Formula:C24H50O4Si2 CAS:104255-99-4 MolWeight:458 RetIndex:2392
CompName:Dodecanedioic acid, 2TBDMS derivative $$ Dodecanedioic acid, bis(tert-butyldimethylsilyl) ester $$ Bis[tert-butyl(dimethyl)silyl] dodecanedic



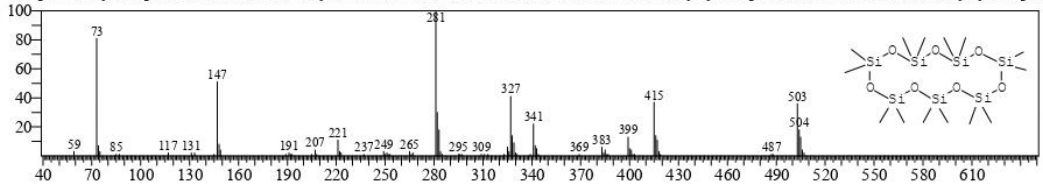
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:50 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



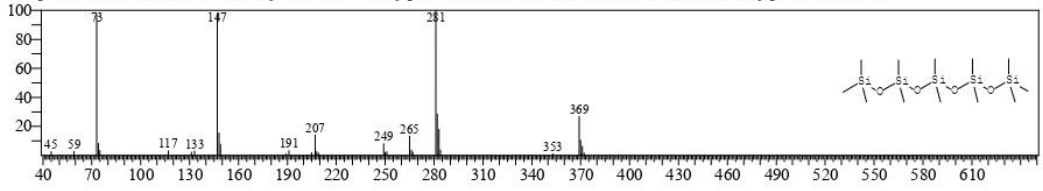
<< Target >>
Line#:23 R.Time:14.645(Scan#:2530) MassPeaks:343
RawMode:Averaged 14.640-14.650(2529-2531) BasePeak:281.05(1620139)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



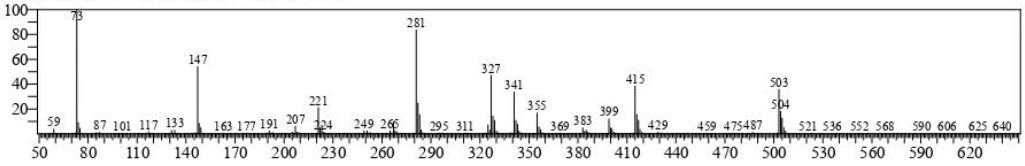
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:93 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



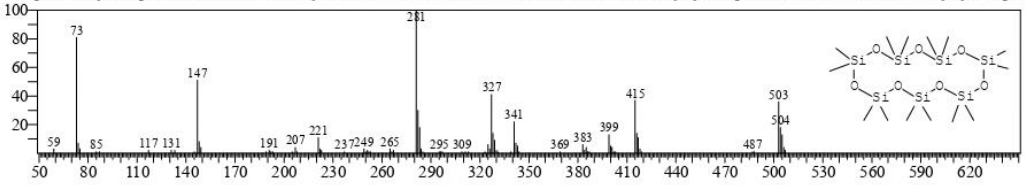
Hit#:2 Entry:37150 Library:NIST17s.lib
SI:58 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane # $$



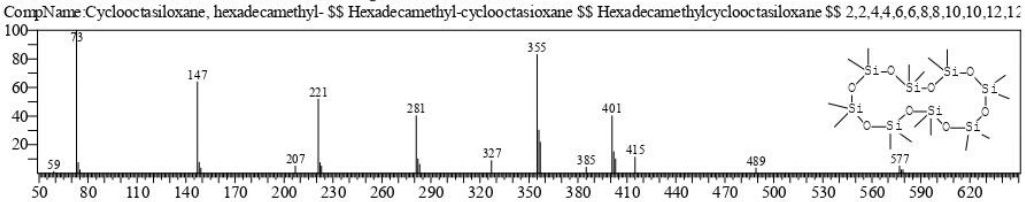
<< Target >>
Line#:24 R.Time:14.875(Scan#:2576) MassPeaks:422
RawMode:Averaged 14.870-14.880(2575-2577) BasePeak:73.05(7010216)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



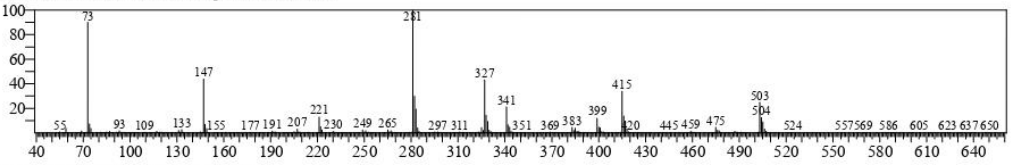
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:93 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



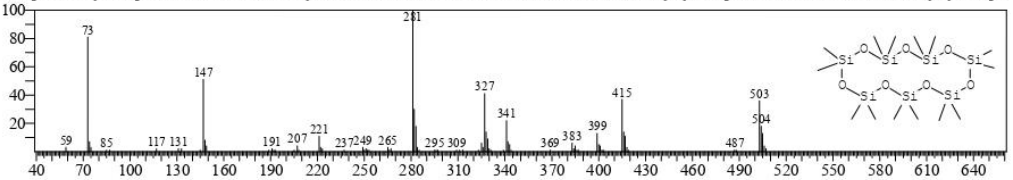
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:64 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



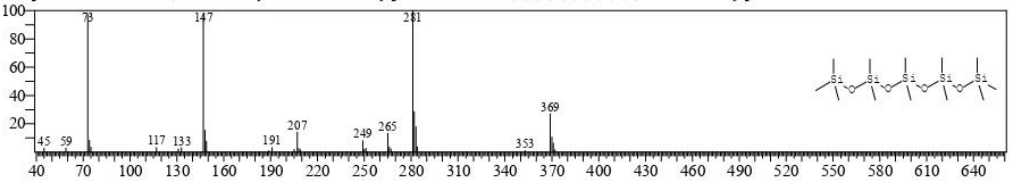
<< Target >>
Line#:25 R.Time:14.955(Scan#:2592) MassPeaks:464
RawMode:Averaged 14.950-14.960(2591-2593) BasePeak:281.05(6658923)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



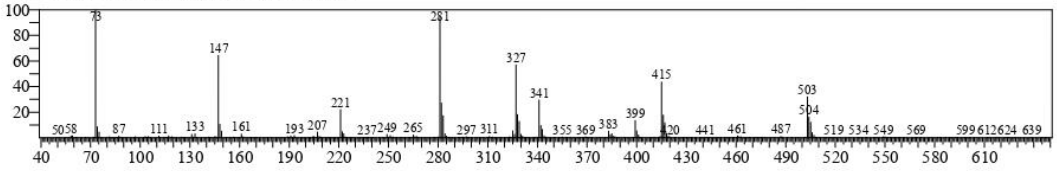
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:96 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



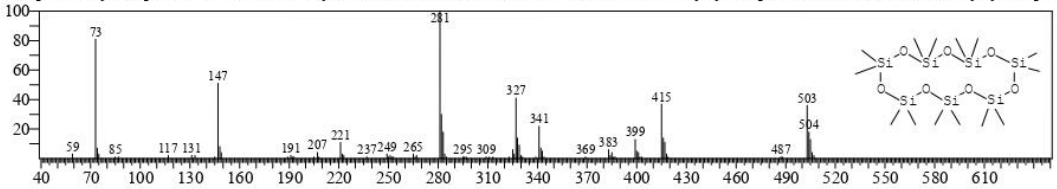
Hit#:2 Entry:37150 Library:NIST17s.lib
SI:64 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane # $$



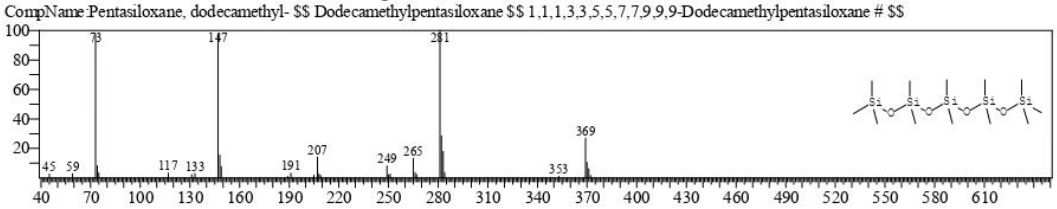
<< Target >>
Line#:26 R.Time:15.250(Scan#:2651) MassPeaks:401
RawMode:Averaged 15.245-15.255(2650-2652) BasePeak:73.05(2176532)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



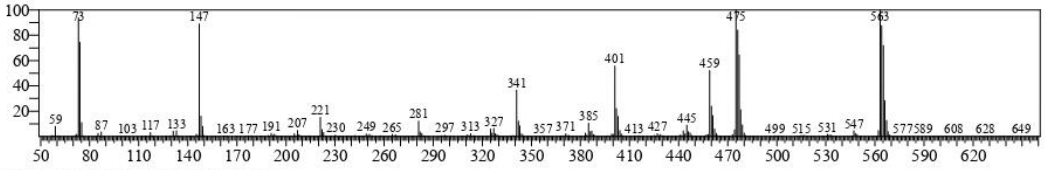
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:94 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcycloheptа



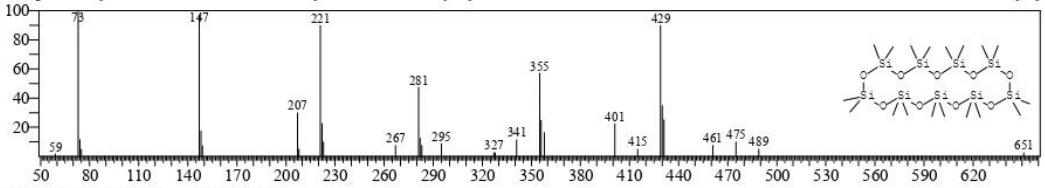
Hit#:2 Entry:37150 Library:NIST17s.lib
SI:62 Formula:C12H36O4Si5 CAS:141-63-9 MolWeight:384 RetIndex:1068
CompName:Pentasiloxane, dodecamethyl- $$ Dodecamethylpentasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,9-Dodecamethylpentasiloxane # $$



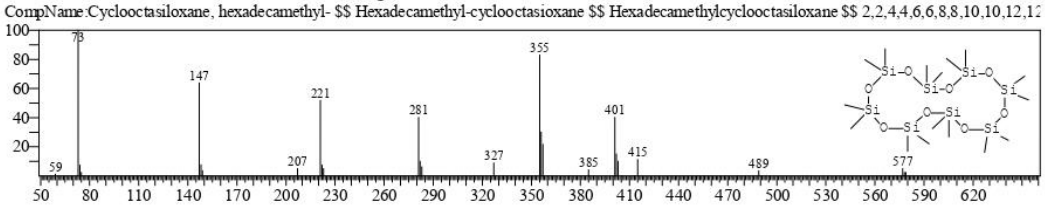
<< Target >>
Line#:27 R.Time:15.415(Scan#:2684) MassPeaks:458
RawMode:Averaged 15.410-15.420(2683-2685) BasePeak:563.15(8246634)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



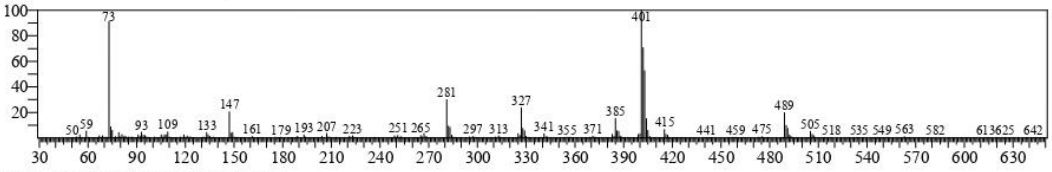
Hit#:1 Entry:39158 Library:NIST17s.lib
SI:42 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



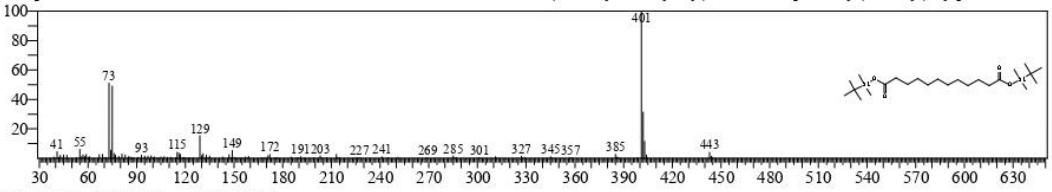
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:40 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,1



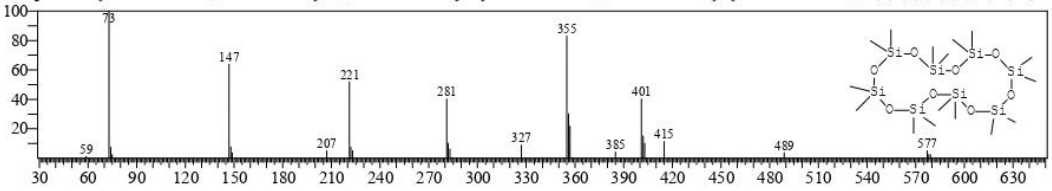
<< Target >>
Line#:28 R.Time:15.670(Scan#:2735) MassPeaks:495
RawMode:Averaged 15.665-15.675(2734-2736) BasePeak:401.05(7248337)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



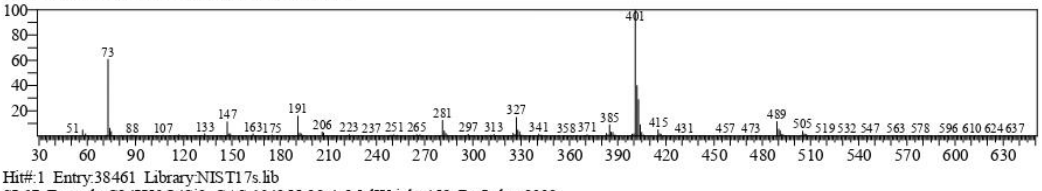
Hit#:1 Entry:38461 Library:NIST17s.lib
SI:61 Formula:C24H50O4Si2 CAS:104255-99-4 MolWeight:458 RetIndex:2392
CompName:Dodecanedioic acid, 2TBDMS derivative $$ Dodecanedioic acid, bis(tert-butyldimethylsilyl) ester $$ Bis[tert-butyl(dimethyl)silyl] dodecanedic



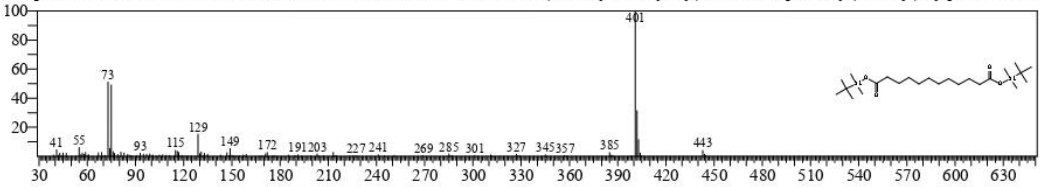
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:58 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



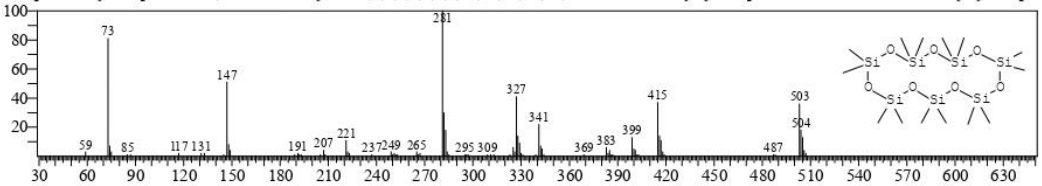
<< Target >>
Line#:29 R.Time:15.730(Scan#:2747) MassPeaks:414
RawMode:Averaged 15.725-15.735(2746-2748) BasePeak:401.00(4360415)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



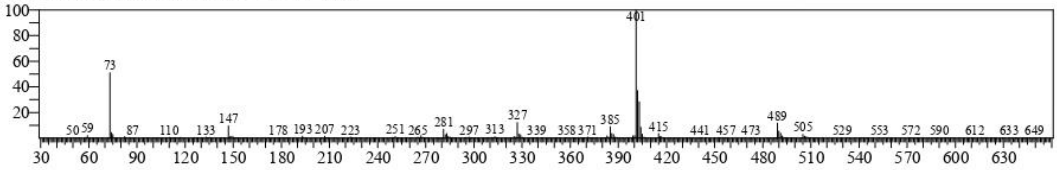
Hit#:1 Entry:38461 Library:NIST17s.lib
SI:67 Formula:C24H50O4Si2 CAS:104255-99-4 MolWeight:458 RetIndex:2392
CompName:Dodecanedioic acid, 2TBDMS derivative $$ Dodecanedioic acid, bis(tert-butyldimethylsilyl) ester $$ Bis[tert-butyl(dimethyl)silyl] dodecanedic



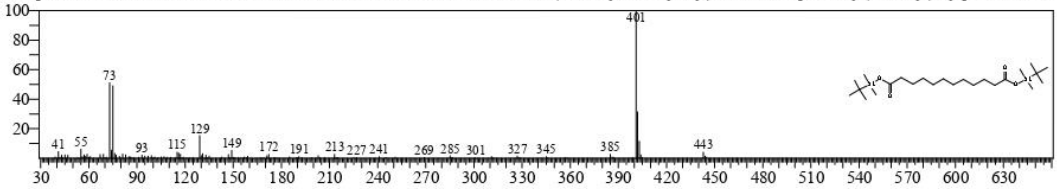
Hit#:2 Entry:38852 Library:NIST17s.lib
SI:55 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



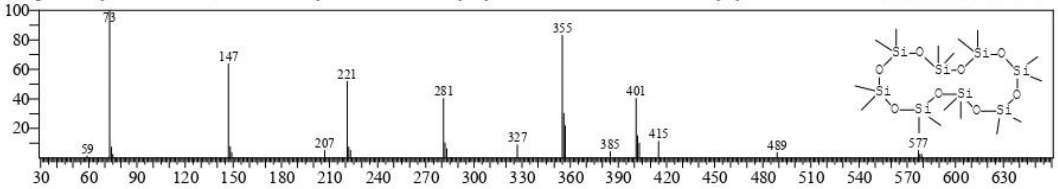
<< Target >>
Line#:30 R.Time:15.775(Scan#:2756) MassPeaks:360
RawMode:Averaged 15.770-15.780(2755-2757) BasePeak:401.00(3562967)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



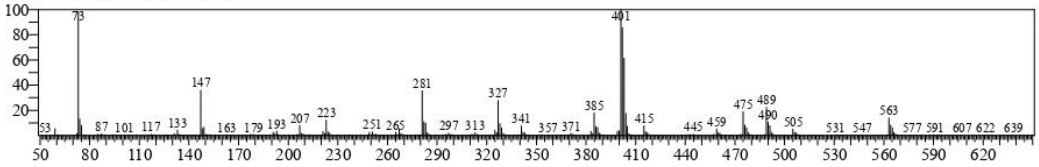
Hit#:1 Entry:38461 Library:NIST17s.lib
SI:69 Formula:C24H50O4Si2 CAS:104255-99-4 MolWeight:458 RetIndex:2392
CompName:Dodecanedioic acid, 2TBDMS derivative $$ Dodecanedioic acid, bis(tert-butyldimethylsilyl) ester $$ Bis[tert-butyl(dimethyl)silyl] dodecanedic



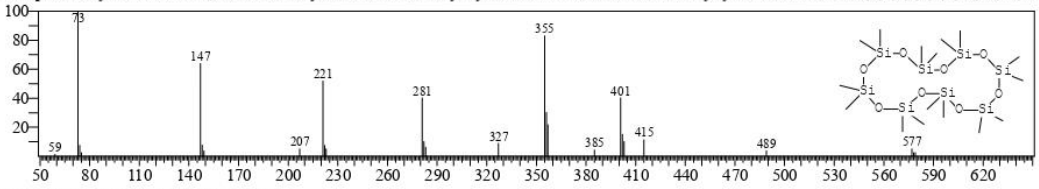
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:54 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



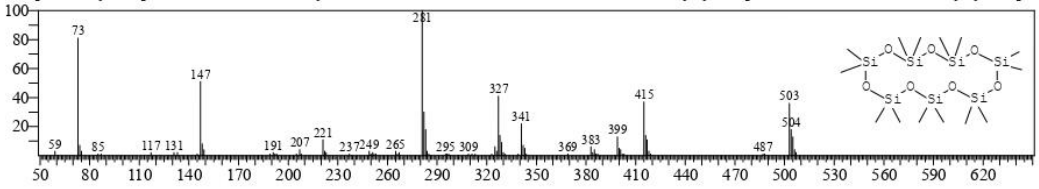
<< Target >>
Line#:31 R.Time:15.855(Scan#:2772) MassPeaks:486
RawMode:Averaged 15.850-15.860(2771-2773) BasePeak:401.05(7399243)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



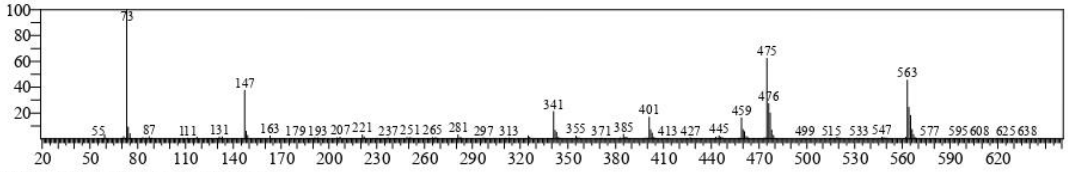
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:61 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



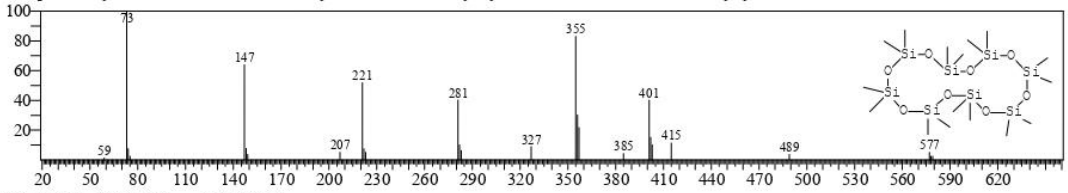
Hit#:2 Entry:38852 Library:NIST17s.lib
SI:58 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



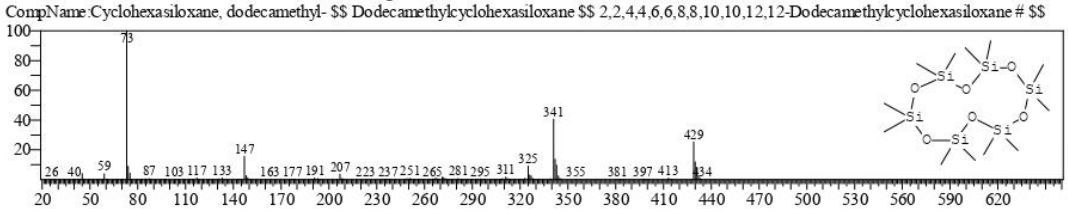
<< Target >>
Line#:32 R.Time:15.925(Scan#:2786) MassPeaks:398
RawMode:Averaged 15.920-15.930(2785-2787) BasePeak:73.05(3068303)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



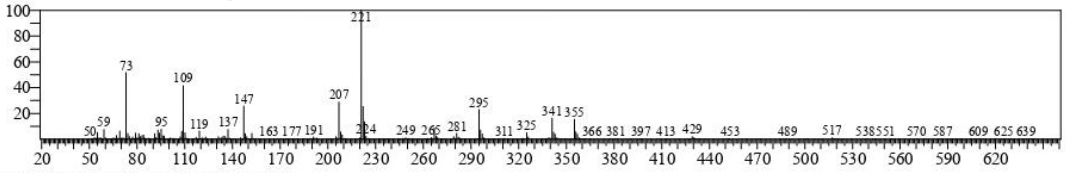
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:49 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



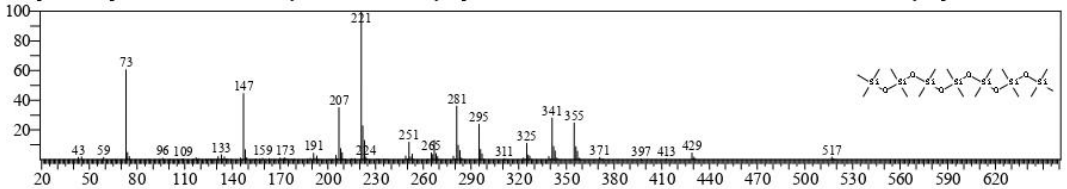
Hit#:2 Entry:38328 Library:NIST17s.lib
SI:49 Formula:C12H36O6Si6 CAS:540-97-6 MolWeight:444 RetIndex:1240
CompName:Cyclohexasiloxane, dodecamethyl- $$ Dodecamethylcyclohexasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12-Dodecamethylcyclohexasiloxane # $$



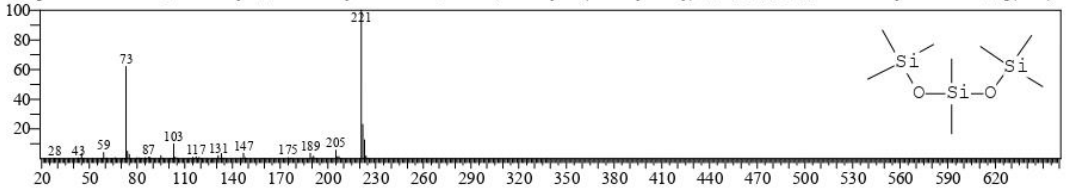
<< Target >>
Line#:33 R.Time:15.990(Scan#:2799) MassPeaks:372
RawMode:Averaged 15.985-15.995(2798-2800) BasePeak:221.05(7165416)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



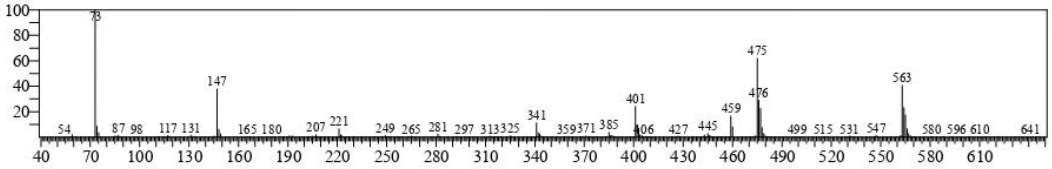
Hit#:1 Entry:38891 Library:NIST17s.lib
SI:75 Formula:C16H48O6Si7 CAS:541-01-5 MolWeight:532 RetIndex:1437
CompName:Heptasiloxane, hexadecamethyl- $$ Hexadecamethylheptasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,13,13,13-Hexadecamethylheptasiloxane # $$



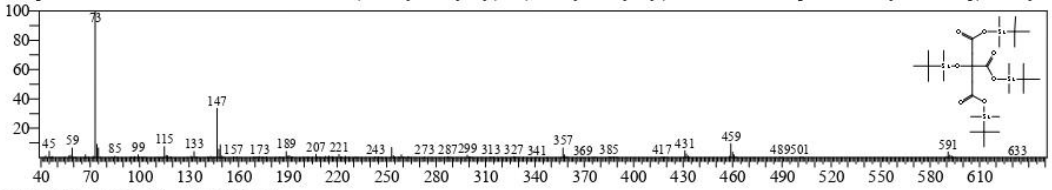
Hit#:2 Entry:27060 Library:NIST17s.lib
SI:61 Formula:C8H24O2Si3 CAS:107-51-7 MolWeight:236 RetIndex:698
CompName:Trisiloxane, octamethyl- $$ Octamethyltrisiloxane $$ Silane, dimethylbis(trimethylsiloxy)- $$ 1,1,1,3,3,5,5,5-Octamethyltrisiloxane $$ [(CH3)3



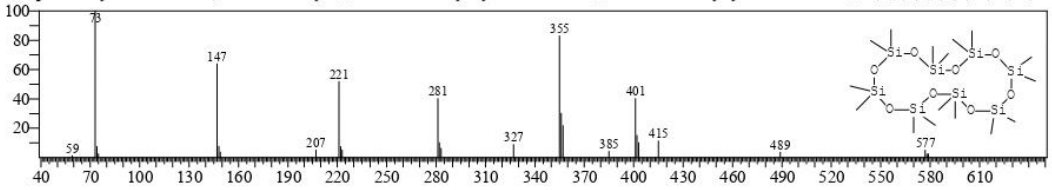
<< Target >>
Line#:34 R.Time:16.295(Scan#:2860) MassPeaks:343
RawMode:Averaged 16.290-16.300(2859-2861) BasePeak:73.05(2583692)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



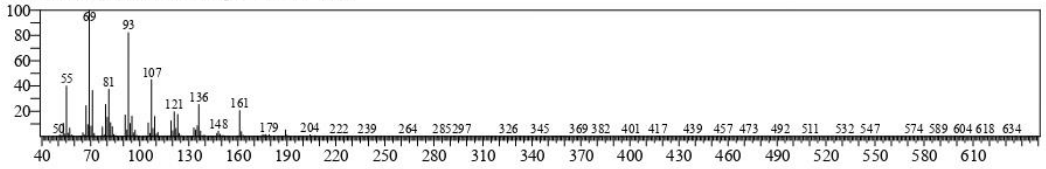
Hit#:1 Entry:39142 Library:NIST17s.lib
SI:49 Formula:C30H64O7Si4 CAS:99477-48-2 MolWeight:648 RetIndex:2799
CompName:Citric acid, 4TBDMS derivative $$ Tris(dimethyl-t-butylsilyl) O-(dimethyl-t-butylsilyl)citrate $$ 1,2,3-Propanetricarboxylic acid, 2-[(tert-butyld



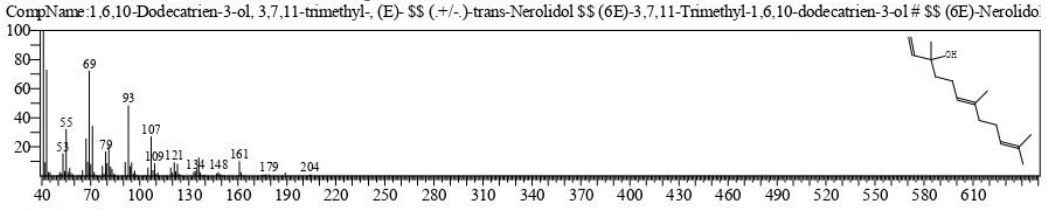
Hit#:2 Entry:39042 Library:NIST17s.lib
SI:48 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



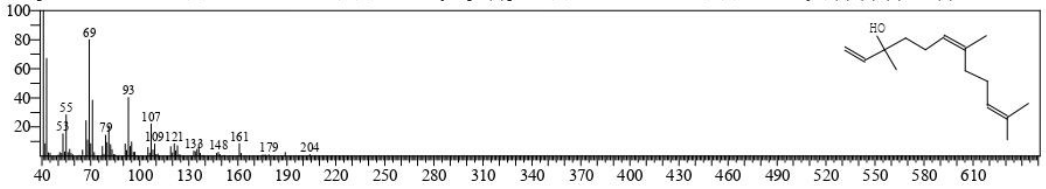
<< Target >>
Line#:35 R.Time:16.475(Scan#:2896) MassPeaks:273
RawMode:Averaged 16.470-16.480(2895-2897) BasePeak:69.05(6440073)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



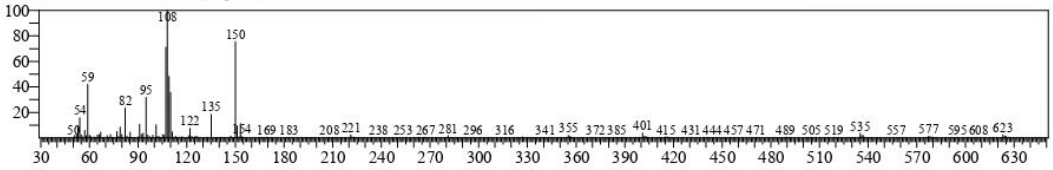
Hit#:1 Entry:25318 Library:NIST17s.lib
SI:93 Formula:C15H26O CAS:40716-66-3 MolWeight:222 RetIndex:1564
CompName:1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)- $$ (.+/-.)-trans-Nerolidol $$ (6E)-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol # $$ (6E)-Nerolidol



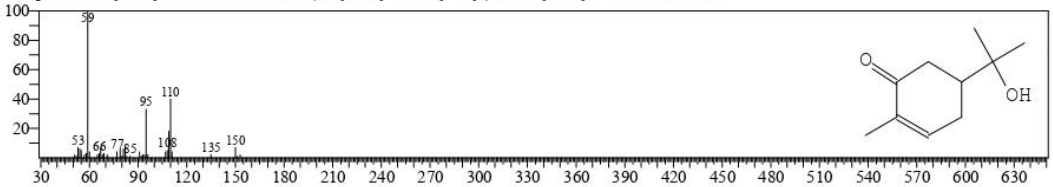
Hit#:2 Entry:25320 Library:NIST17s.lib
SI:91 Formula:C15H26O CAS:142-50-7 MolWeight:222 RetIndex:1564
CompName:Nerolidol $$ 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, [S-(Z)]- $$ 1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (Z)-(S)-(+)- $$ (+)-Nerolidol $$



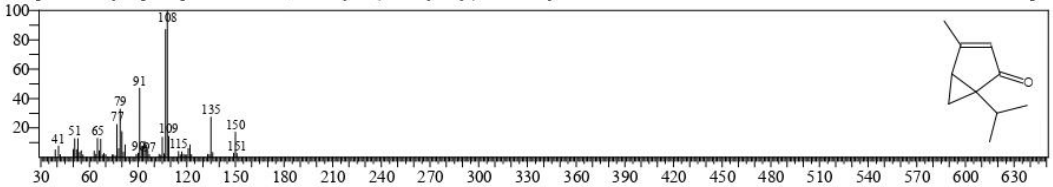
<< Target >>
Line#:36 R.Time:16.565(Scan#:2914) MassPeaks:354
RawMode:Averaged 16.560-16.570(2913-2915) BasePeak:108.10(2253143)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



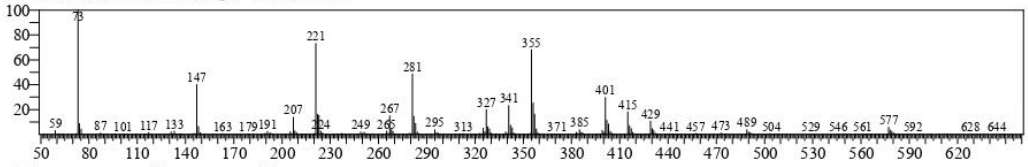
Hit#:1 Entry:15012 Library:NIST17s.lib
SI:70 Formula:C10H16O2 CAS:7712-46-1 MolWeight:168 RetIndex:1314
CompName:8-Hydroxycarvotanacetone $$ 5-(1-Hydroxy-1-methylethyl)-2-methyl-2-cyclohexen-1-one # $$



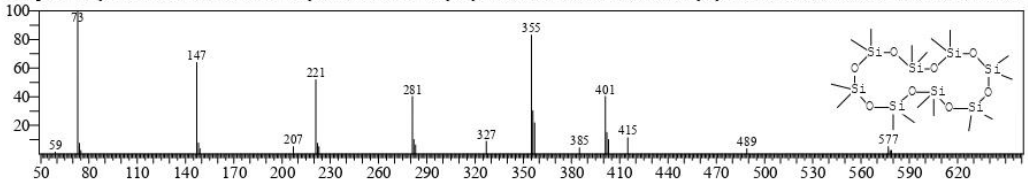
Hit#:2 Entry:10838 Library:NIST17s.lib
SI:68 Formula:C10H14O CAS:24545-81-1 MolWeight:150 RetIndex:1073
CompName:Bicyclo[3.1.0]hex-3-en-2-one, 4-methyl-1-(1-methylethyl)- $$ 3-Thujen-2-one $$ Umbellulon $$ Umbellulone $$ THUJEN-2-ONE $$ 1-Isopro



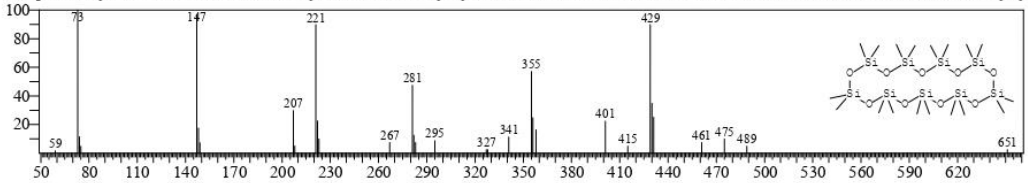
<< Target >>
Line#:37 R.Time:16.960(Scan#:2993) MassPeaks:394
RawMode:Averaged 16.955-16.965(2992-2994) BasePeak:73.05(6090358)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



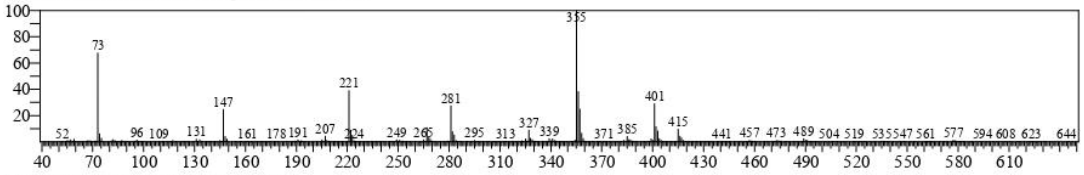
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:83 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



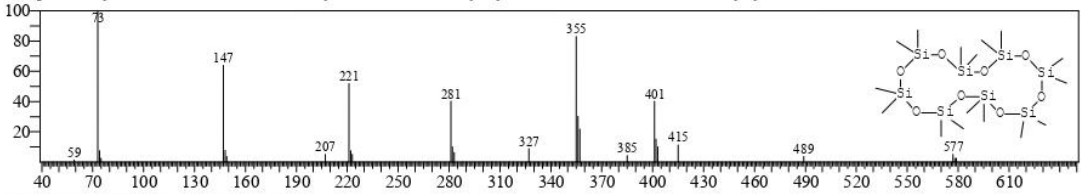
Hit#:2 Entry:39158 Library:NIST17s.lib
SI:79 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



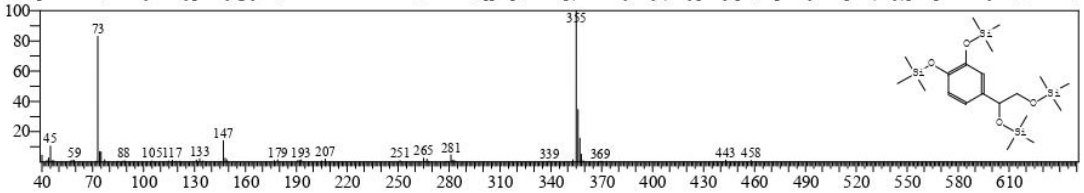
<< Target >>
Line#:38 R.Time:17.150(Scan#:3031) MassPeaks:435
RawMode:Averaged 17.145-17.155(3030-3032) BasePeak:355.05(7094632)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



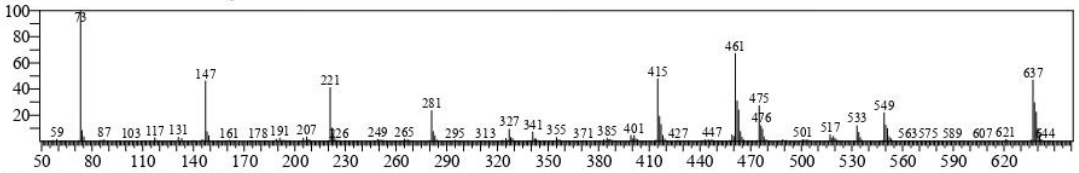
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:86 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



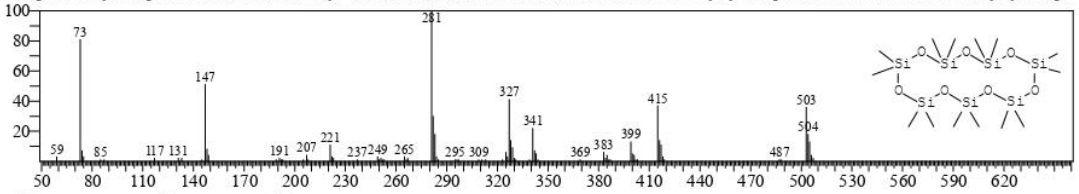
Hit#:2 Entry:38459 Library:NIST17s.lib
SI:72 Formula:C20H42O4Si4 CAS:56114-62-6 MolWeight:458 RetIndex:1993
CompName:3,4-Dihydroxyphenylglycol, 4TMS derivative $$ Silane, [[4-[1,2-bis[(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(oxy)]bis[trimethyl- $$ Silane,



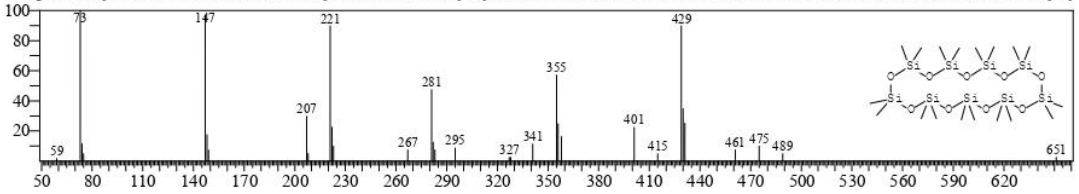
<< Target >>
Line#:39 R.Time:17.360(Scan#:3073) MassPeaks:437
RawMode:Averaged 17.355-17.365(3072-3074) BasePeak:73.05(1905748)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



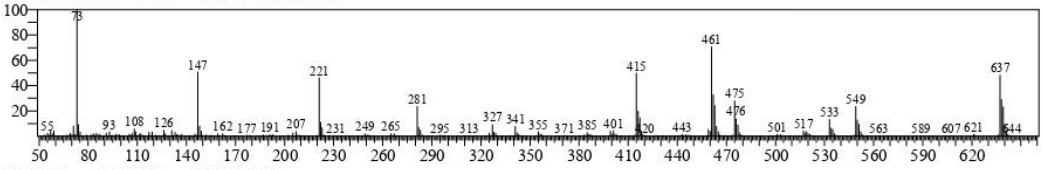
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:53 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



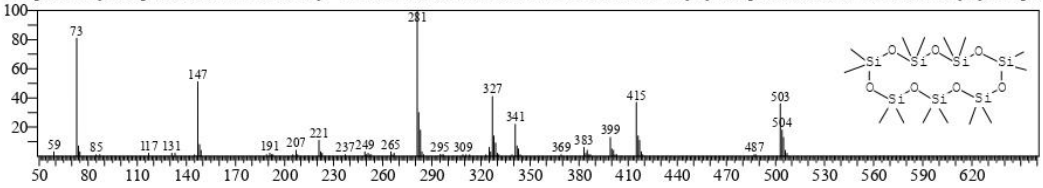
Hit#:2 Entry:39158 Library:NIST17s.lib
SI:52 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



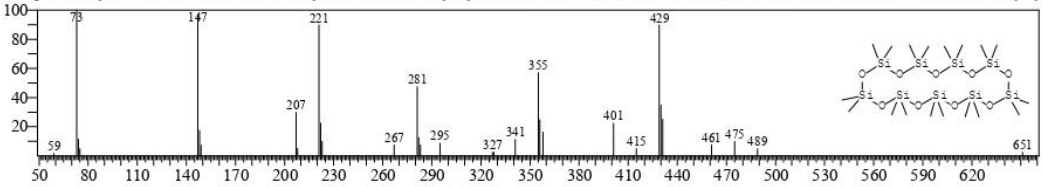
<< Target >>
Line#:40 R.Time:17.515(Scan#:3104) MassPeaks:477
RawMode:Averaged 17.510-17.520(3103-3105) BasePeak:73.05(2444563)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



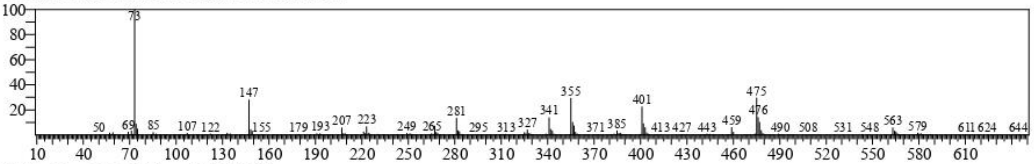
Hit#:1 Entry:38852 Library:NIST17s.lib
SI:51 Formula:C14H42O7Si7 CAS:107-50-6 MolWeight:518 RetIndex:1447
CompName:Cycloheptasiloxane, tetradecamethyl- $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane # $$ Tetradecamethylcyclohepta



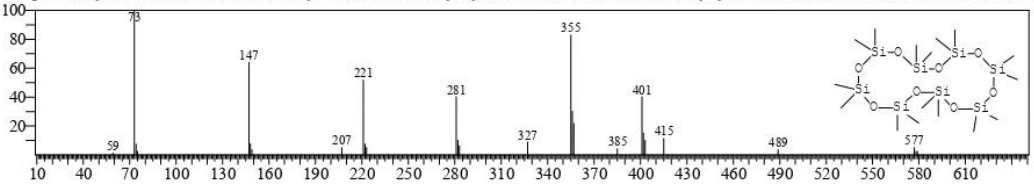
Hit#:2 Entry:39158 Library:NIST17s.lib
SI:49 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



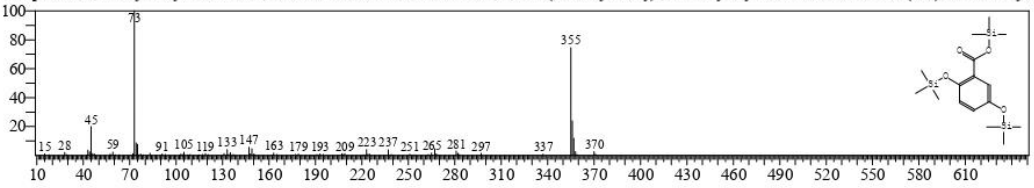
<< Target >>
Line#:41 R.Time:17.765(Scan#:3154) MassPeaks:388
RawMode:Averaged 17.760-17.770(3153-3155) BasePeak:73.05(3539835)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



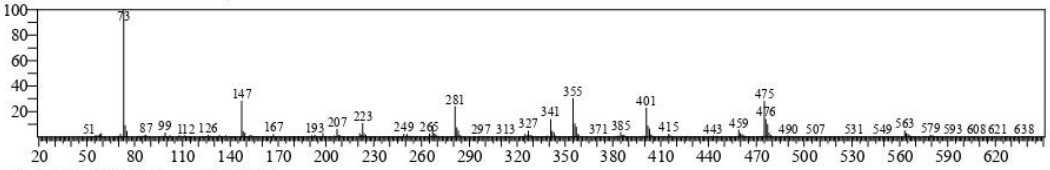
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:70 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



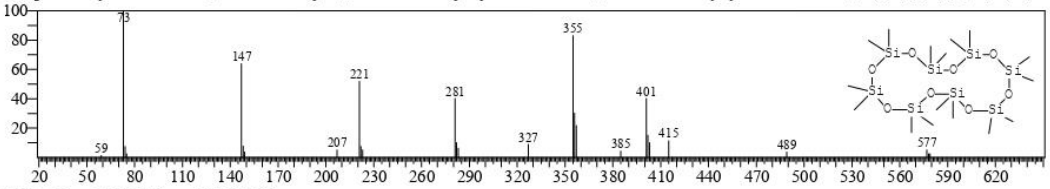
Hit#:2 Entry:36734 Library:NIST17s.lib
SI:64 Formula:C16H30O4Si3 CAS:3618-20-0 MolWeight:370 RetIndex:1765
CompName:2,5-Dihydroxybenzoic acid, 3TMS derivative $$ Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester $$ Gentisic acid (tms) $$ Trimethyl



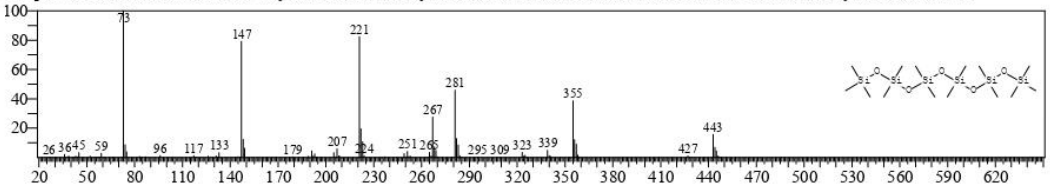
<< Target >>
Line#:42 R.Time:17.940(Scan#:3189) MassPeaks:460
RawMode:Averaged 17.935-17.945(3188-3190) BasePeak:73.05(3995758)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



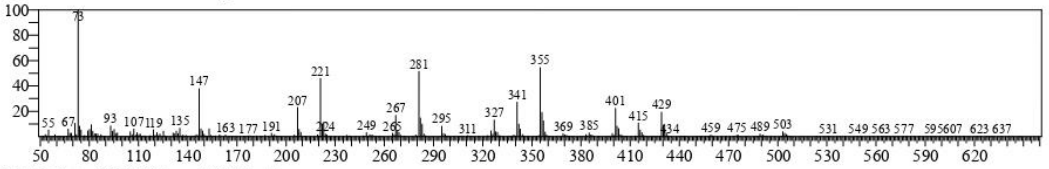
Hit#:1 Entry:39042 Library:NIST17s.lib
SI:72 Formula:C16H48O8Si8 CAS:556-68-3 MolWeight:592 RetIndex:1654
CompName:Cyclooctasiloxane, hexadecamethyl- $$ Hexadecamethyl-cyclooctasioxane $$ Hexadecamethylcyclooctasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12



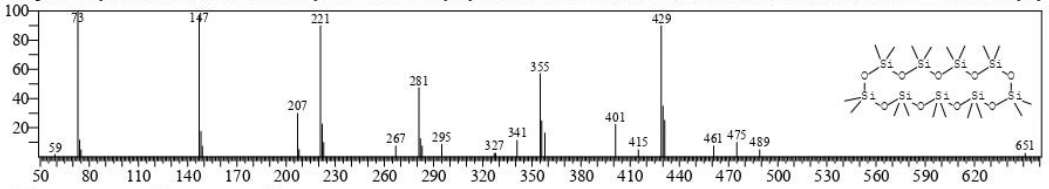
Hit#:2 Entry:38451 Library:NIST17s.lib
SI:66 Formula:C14H42O5Si6 CAS:107-52-8 MolWeight:458 RetIndex:1252
CompName:Hexasiloxane, tetradecamethyl- $$ Tetradecamethylhexasiloxane $$ 1,1,1,3,3,5,5,7,7,9,9,11,11,11-Tetradecamethylhexasiloxane # $$



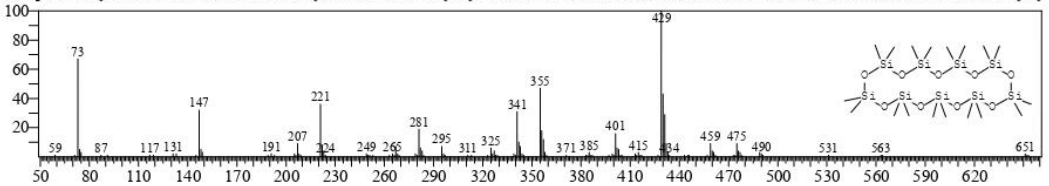
<< Target >>
Line#:43 R.Time:19.055(Scan#:3412) MassPeaks:406
RawMode:Averaged 19.050-19.060(3411-3413) BasePeak:73.05(1179367)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



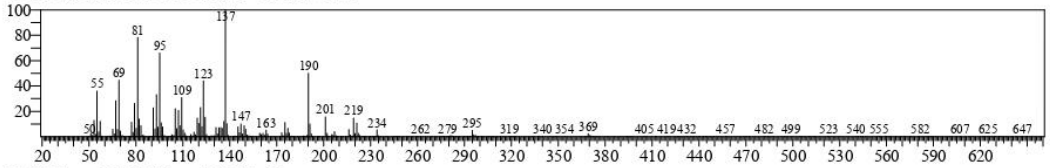
Hit#:1 Entry:39158 Library:NIST17s.lib
SI:76 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



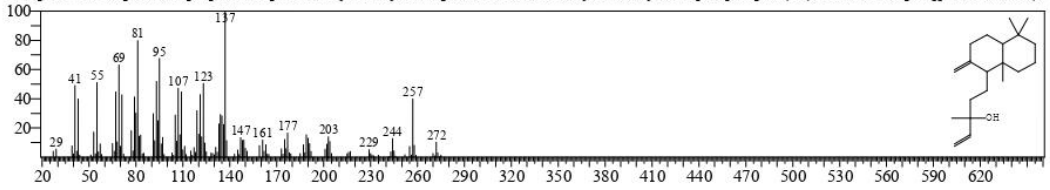
Hit#:2 Entry:39159 Library:NIST17s.lib
SI:75 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



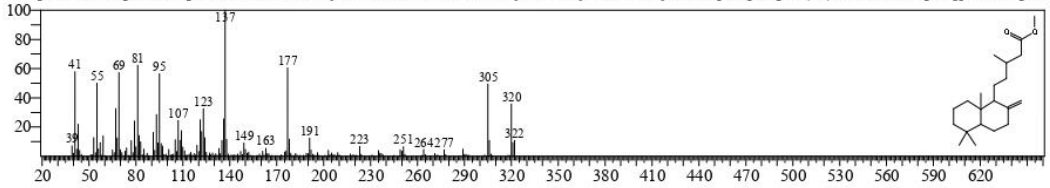
<< Target >>
Line#:44 R.Time:20.055(Scan#:3612) MassPeaks:319
RawMode:Averaged 20.050-20.060(3611-3613) BasePeak:137.15(1757011)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



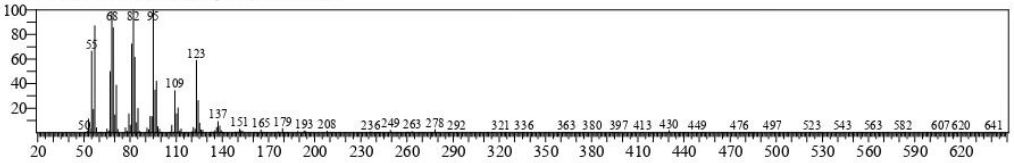
Hit#:1 Entry:32335 Library:NIST17s.lib
SI:79 Formula:C20H34O CAS:1438-62-6 MolWeight:290 RetIndex:2016
CompName:1-Naphthalenepropanol, .alpha.-ethenyldecahydro-.alpha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.(R*),4a.beta.,8a.alpha.]]- $$ Labda-8(2



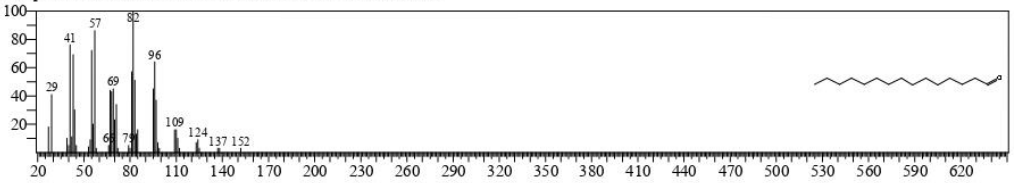
Hit#:2 Entry:34367 Library:NIST17s.lib
SI:76 Formula:C21H36O2 CAS:13008-80-5 MolWeight:320 RetIndex:2137
CompName:1-Naphthalenepentanoic acid, decahydro-.beta.,5,5,8a-tetramethyl-2-methylene-, methyl ester, [1R-[1.alpha.(S*),4a.beta.,8a.alpha.]]- $$ Ladp-8(



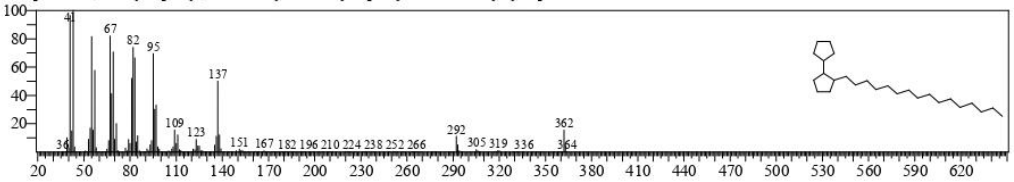
<< Target >>
Line#:45 R.Time:20.150(Scan#:3631) MassPeaks:258
RawMode:Averaged 20.145-20.155(3630-3632) BasePeak:82.10(1184957)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



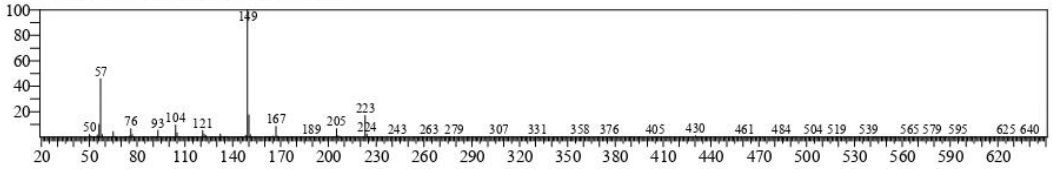
Hit#:1 Entry:25974 Library:NIST17s.lib
SI:87 Formula:C15H30O CAS:2765-11-9 MolWeight:226 RetIndex:1701
CompName:Pentadecanal- $$ 1-Pentadecanal $$ n-Pentadecanal $$



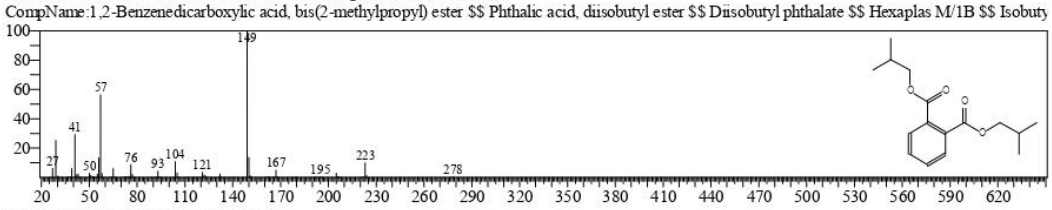
Hit#:2 Entry:36487 Library:NIST17s.lib
SI:86 Formula:C26H50 CAS:55334-11-7 MolWeight:362 RetIndex:2653
CompName:1,1'-Bicyclopentyl, 2-hexadecyl- $$ 1-Cyclopentyl-2-n-hexadecylcyclopentane $$



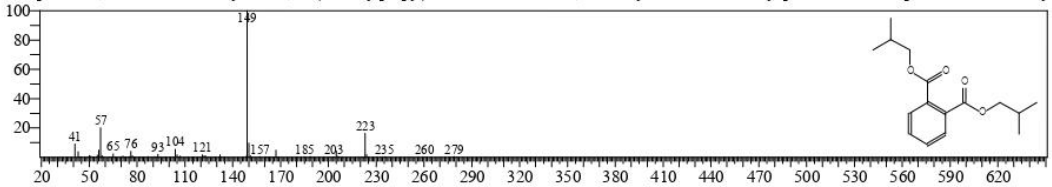
<< Target >>
Line#:46 R.Time:20.535(Scan#:3708) MassPeaks:310
RawMode:Averaged 20.530-20.540(3707-3709) BasePeak:149.15(7935340)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



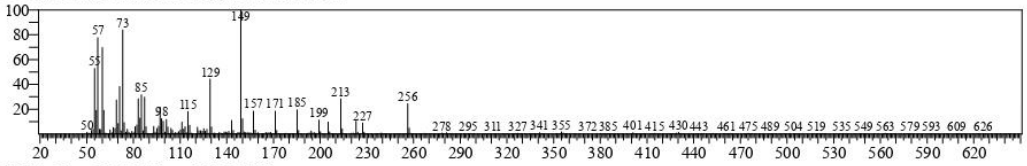
Hit#:1 Entry:31271 Library:NIST17s.lib
SI:94 Formula:C16H22O4 CAS:84-69-5 MolWeight:278 RetIndex:1908
CompName:1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester $$ Phthalic acid, diisobutyl ester $$ Diisobutyl phthalate $$ Hexaplas M/1B $$ Isobuty



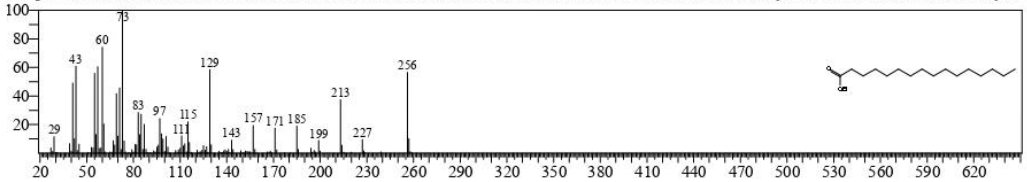
Hit#:2 Entry:31275 Library:NIST17s.lib
SI:90 Formula:C16H22O4 CAS:84-69-5 MolWeight:278 RetIndex:1908
CompName:1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester $$ Phthalic acid, diisobutyl ester $$ Diisobutyl phthalate $$ Hexaplas M/1B $$ Isobuty



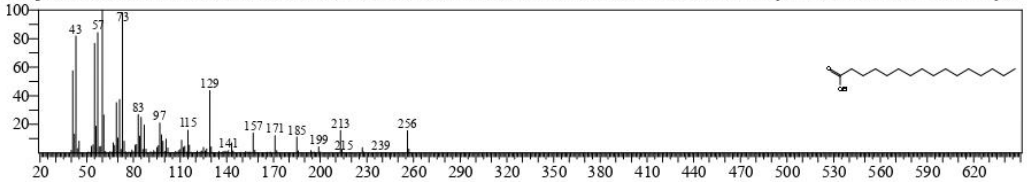
<< Target >>
Line#:47 R.Time:21.710(Scan#:3943) MassPeaks:452
RawMode:Averaged 21.705-21.715(3942-3944) BasePeak:149.05(7718524)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



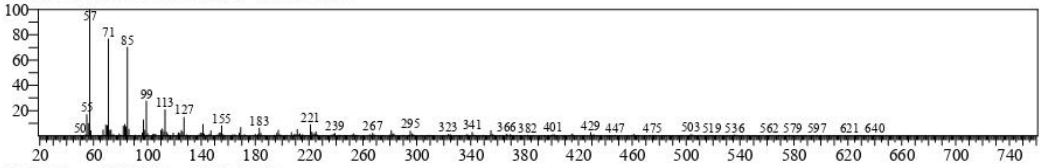
Hit#:1 Entry:29350 Library:NIST17s.lib
SI:87 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



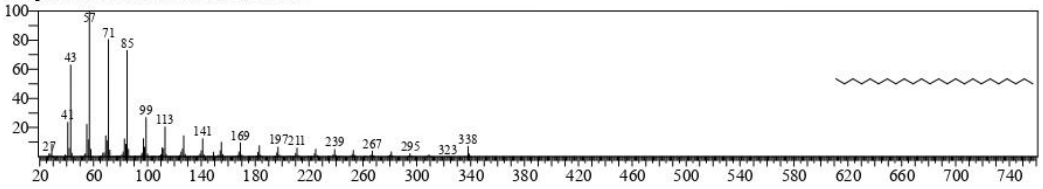
Hit#:2 Entry:29349 Library:NIST17s.lib
SI:85 Formula:C16H32O2 CAS:57-10-3 MolWeight:256 RetIndex:1968
CompName:n-Hexadecanoic acid $$ Hexadecanoic acid $$ n-Hexadecoic acid $$ Palmitic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic



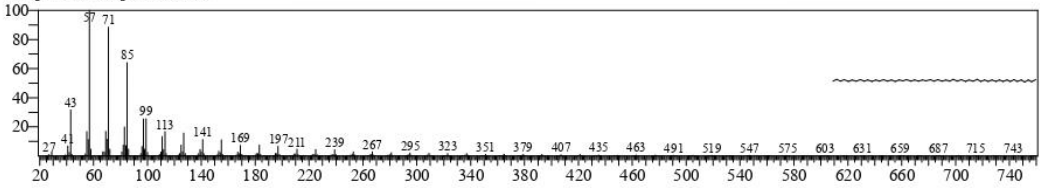
<< Target >>
Line#:48 R.Time:22.585(Scan#:4118) MassPeaks:343
RawMode:Averaged 22.580-22.590(4117-4119) BasePeak:57.10(777913)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



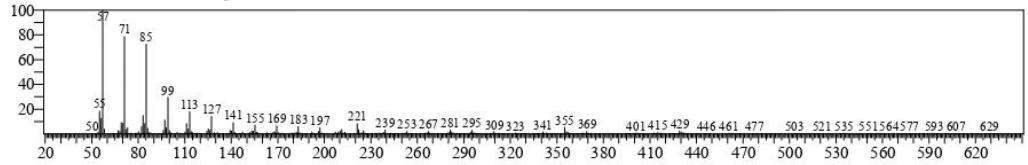
Hit#:1 Entry:35410 Library:NIST17s.lib
SI:90 Formula:C24H50 CAS:646-31-1 MolWeight:338 RetIndex:2407
CompName:Tetracosane $$ n-Tetracosane $$



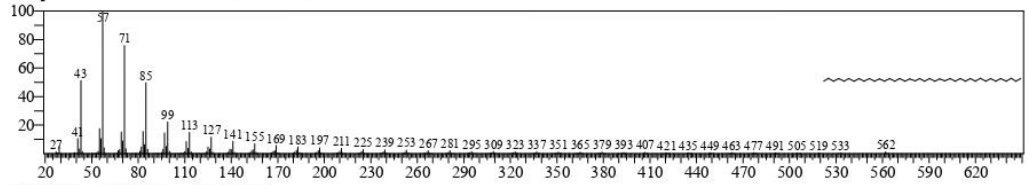
Hit#:2 Entry:39209 Library:NIST17s.lib
SI:90 Formula:C54H110 CAS:5856-66-6 MolWeight:758 RetIndex:5389
CompName:Tetrapentacontane



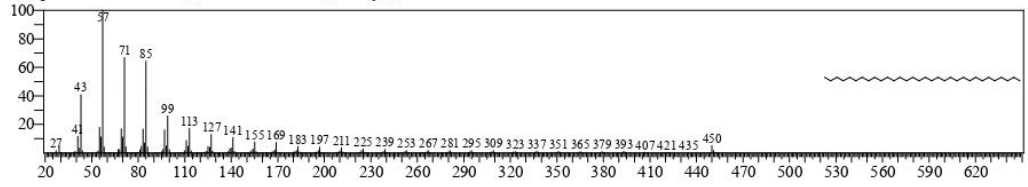
<< Target >>
Line#:49 R.Time:22.645(Scan#:4130) MassPeaks:366
RawMode:Averaged 22.640-22.650(4129-4131) BasePeak:57.10(1083269)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



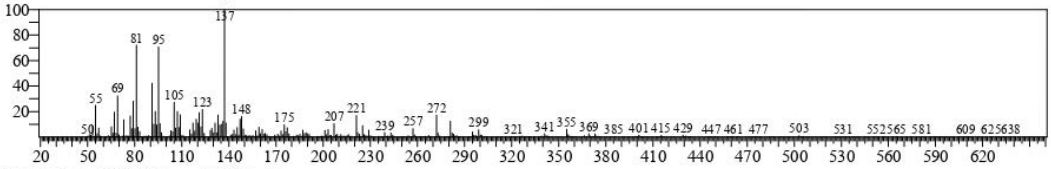
Hit#:1 Entry:38991 Library:NIST17s.lib
SI:93 Formula:C40H82 CAS:4181-95-7 MolWeight:562 RetIndex:3997
CompName:Tetracontane $$ n-Tetracontane $$



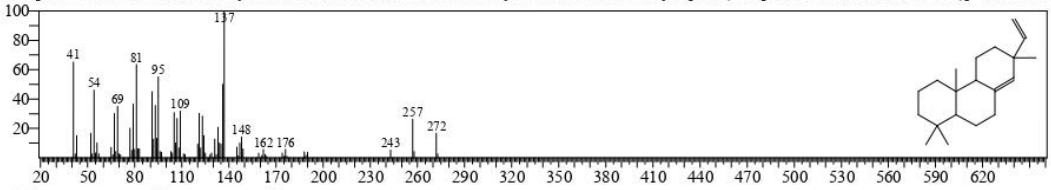
Hit#:2 Entry:38391 Library:NIST17s.lib
SI:92 Formula:C32H66 CAS:544-85-4 MolWeight:450 RetIndex:3202
CompName:Dotriacontane $$ n-Dotriacontane $$ Bicetyl $$



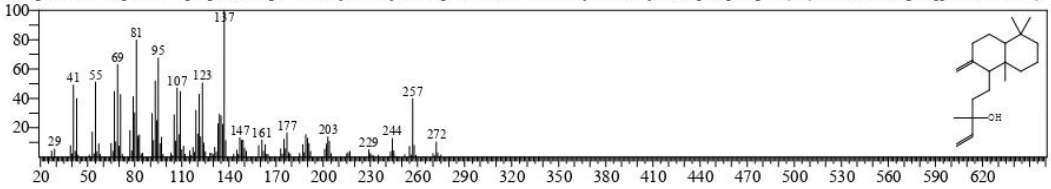
<< Target >>
Line#:50 R.Time:22.990(Scan#:4199) MassPeaks:425
RawMode:Averaged 22.985-22.995(4198-4200) BasePeak:137.15(1240275)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



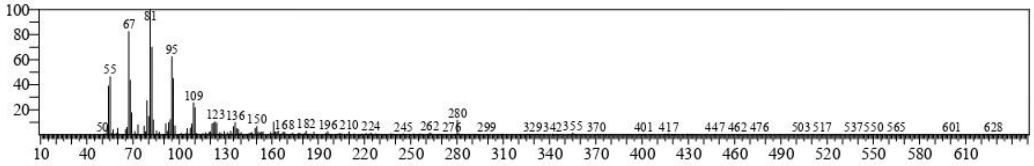
Hit#:1 Entry:30809 Library:NIST17s.lib
SI:79 Formula:C20H32 CAS:1686-56-2 MolWeight:272 RetIndex:1926
CompName:Phenanthrene, 7-ethenyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-, [4aS-(4a.alpha.,4b.beta.,7.beta.,10a.beta.)]- $$ Podoc



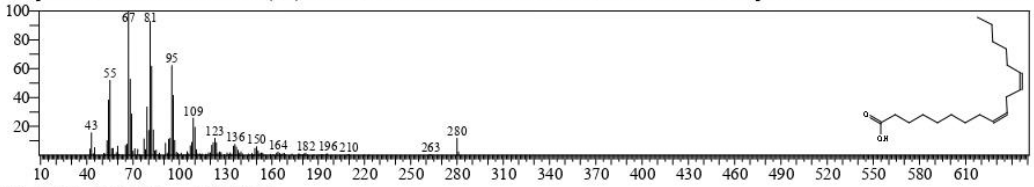
Hit#:2 Entry:32335 Library:NIST17s.lib
SI:75 Formula:C20H34O CAS:1438-62-6 MolWeight:290 RetIndex:2016
CompName:1-Naphthalenepropanol, .alpha.-ethenyldecahydro-.alpha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.(R*),4a.beta.,8a.alpha.]]- $$ Labda-8(2



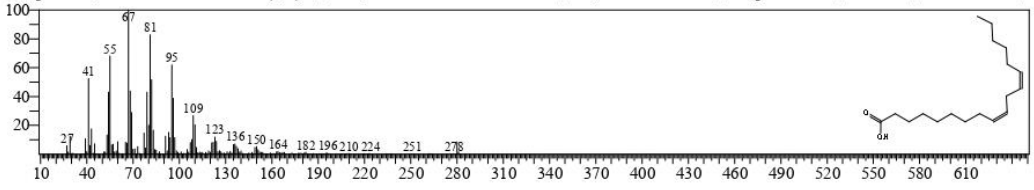
<< Target >>
Line#:51 R.Time:23.665(Scan#:4334) MassPeaks:378
RawMode:Averaged 23.660-23.670(4333-4335) BasePeak:81.10(1571873)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



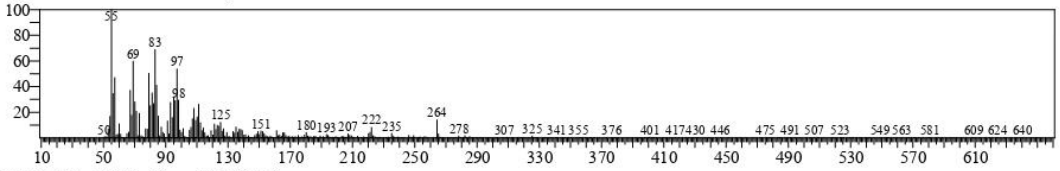
Hit#:1 Entry:31427 Library:NIST17s.lib
SI:93 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $



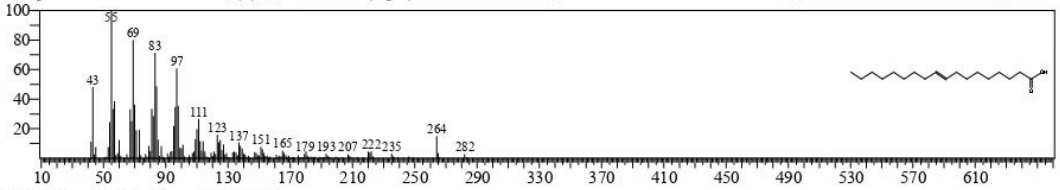
Hit#:2 Entry:31426 Library:NIST17s.lib
SI:91 Formula:C18H32O2 CAS:60-33-3 MolWeight:280 RetIndex:2183
CompName:9,12-Octadecadienoic acid (Z,Z)- $$ cis-9,cis-12-Octadecadienoic acid $$ cis,cis-Linoleic acid $$ Grape seed oil $$ Linoleic $$ Linoleic acid $



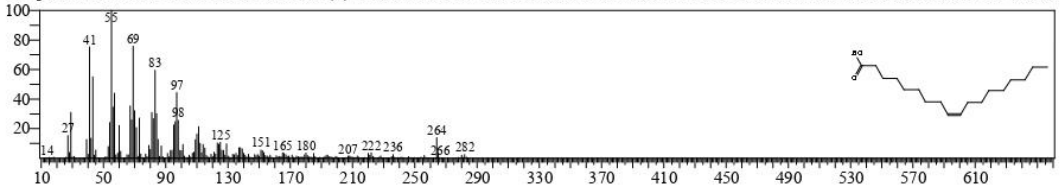
<< Target >>
Line#:52 R.Time:23.735(Scan#:4348) MassPeaks:427
RawMode:Averaged 23.730-23.740(4347-4349) BasePeak:55.05(3950907)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



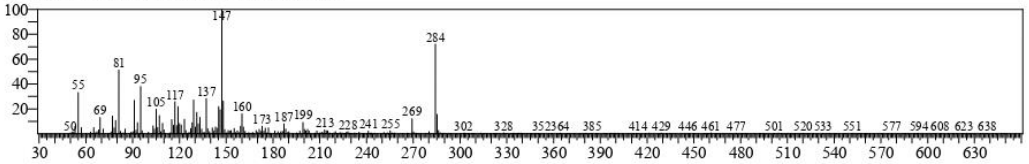
Hit#:1 Entry:31601 Library:NIST17s.lib
SI:87 Formula:C18H34O2 CAS:112-79-8 MolWeight:282 RetIndex:2175
CompName:9-Octadecenoic acid, (E)- $$ trans- delta.(sup 9)-Octadecenoic acid $$ trans- delta.9-Octadecenoic acid $$ trans-Octadec-9-enoic acid $$ trans-



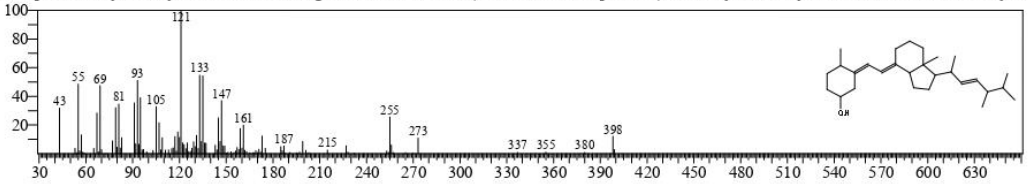
Hit#:2 Entry:31598 Library:NIST17s.lib
SI:87 Formula:C18H34O2 CAS:112-80-1 MolWeight:282 RetIndex:2175
CompName:Oleic Acid $$ 9-Octadecenoic acid (Z)- $$ .DELTA.9-cis-Oleic acid $$ cis-Oleic Acid $$ cis-9-Octadecenoic Acid $$ Emersol 211 $$ Emersol



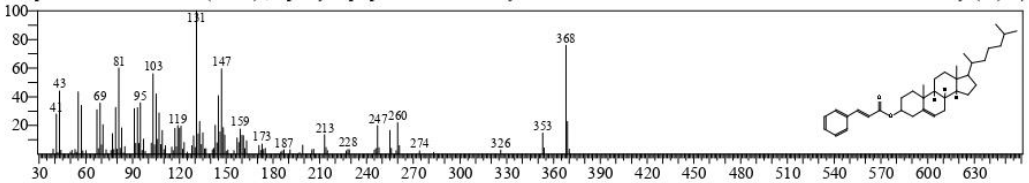
<< Target >>
Line#:53 R.Time:23.820(Scan#:4365) MassPeaks:355
RawMode:Averaged 23.815-23.825(4364-4366) BasePeak:147.10(708257)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



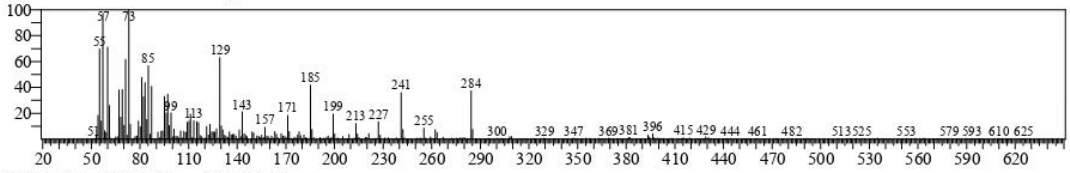
Hit#:1 Entry:37611 Library:NIST17s.lib
SI:62 Formula:C28H46O CAS:67-96-9 MolWeight:398 RetIndex:2843
CompName:Dihydrotachysterol $$ 9,10-Secoergosta-5,7,22-trien-3-ol, (3.beta.,5E,7E,10.alpha.,22E)- $$ Tachysterol, dihydro- $$ A.T. 10 $$ Anti-Tetany st



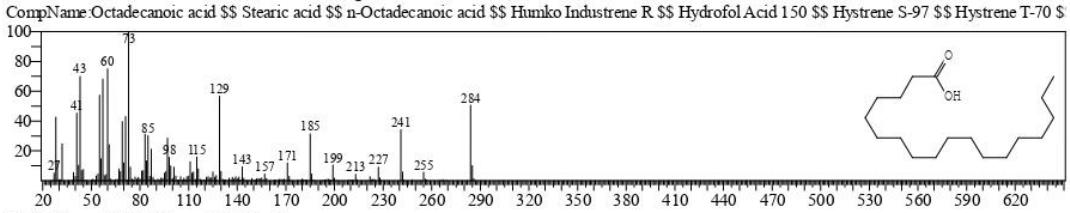
Hit#:2 Entry:38849 Library:NIST17s.lib
SI:62 Formula:C36H52O2 CAS:1990-11-0 MolWeight:516 RetIndex:3516
CompName:Cholest-5-en-3-ol (3.beta.)-, 3-phenyl-2-propenoate $$ Cholesteryl cinnamate $$ 5-Cholesten-3.beta.-ol cinnamate $$ Cholest-5-en-3-yl (2E)-3-



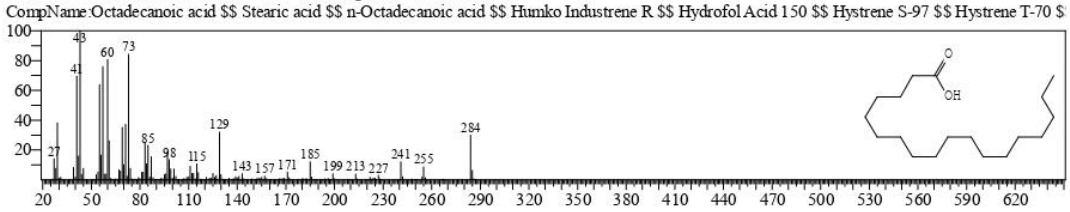
<< Target >>
Line#:54 R.Time:23.955(Scan#:4392) MassPeaks:372
RawMode:Averaged 23.950-23.960(4391-4393) BasePeak:73.05(541927)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



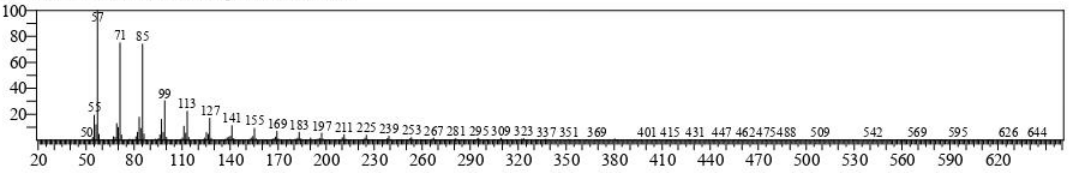
Hit#:1 Entry:31781 Library:NIST17s.lib
SI:85 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



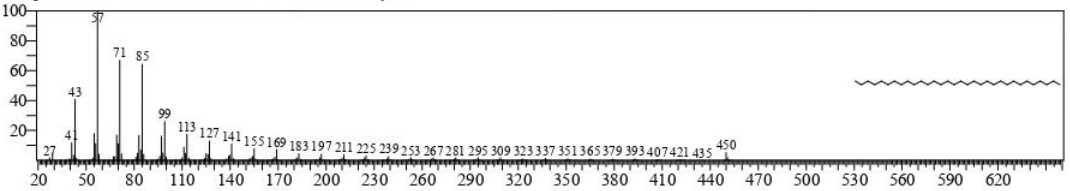
Hit#:2 Entry:31775 Library:NIST17s.lib
SI:82 Formula:C18H36O2 CAS:57-11-4 MolWeight:284 RetIndex:2167
CompName:Octadecanoic acid $$ Stearic acid $$ n-Octadecanoic acid $$ Humko Industrene R $$ Hydrofol Acid 150 $$ Hystrene S-97 $$ Hystrene T-70 $



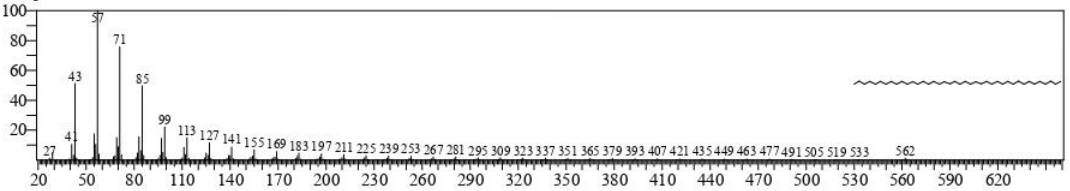
<< Target >>
Line#:55 R.Time:25.080(Scan#:4617) MassPeaks:346
RawMode:Averaged 25.075-25.085(4616-4618) BasePeak:57.05(4334898)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



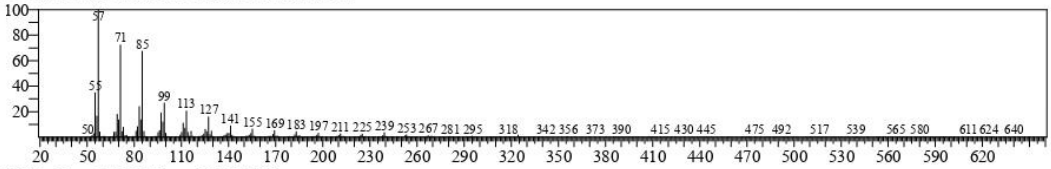
Hit#:1 Entry:38391 Library:NIST17s.lib
SI:95 Formula:C32H66 CAS:544-85-4 MolWeight:450 RetIndex:3202
CompName:Dotriacontane $$ n-Dotriacontane $$ Bicetyl $$



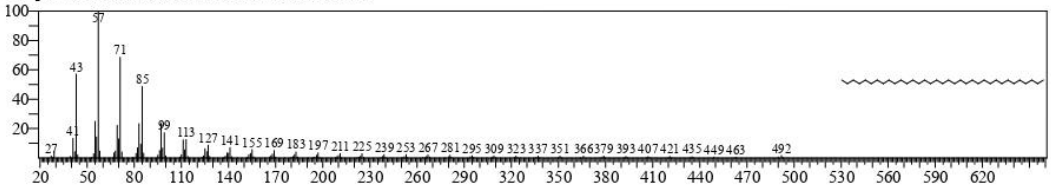
Hit#:2 Entry:38991 Library:NIST17s.lib
SI:95 Formula:C40H82 CAS:4181-95-7 MolWeight:562 RetIndex:3997
CompName:Tetracontane $$ n-Tetracontane $$



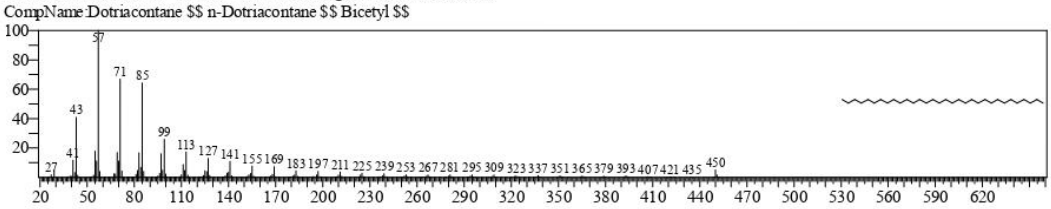
<< Target >>
Line#:56 R.Time:25.325(Scan#:4666) MassPeaks:367
RawMode:Averaged 25.320-25.330(4665-4667) BasePeak:57.05(6434337)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



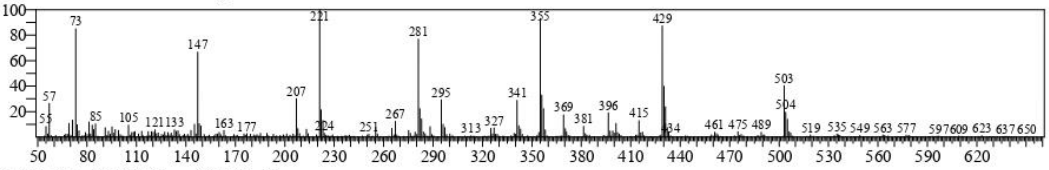
Hit#:1 Entry:38741 Library:NIST17s.lib
SI:93 Formula:C35H72 CAS:630-07-9 MolWeight:492 RetIndex:3500
CompName:Pentatriacontane $$ n-Pentatriacontane $$



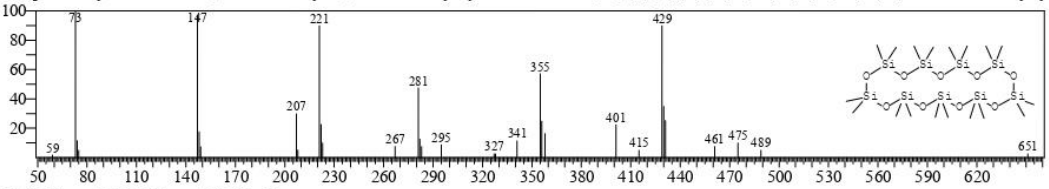
Hit#:2 Entry:38391 Library:NIST17s.lib
SI:92 Formula:C32H66 CAS:544-85-4 MolWeight:450 RetIndex:3202
CompName:Dotriacontane $$ n-Dotriacontane $$ Bicetyl $$



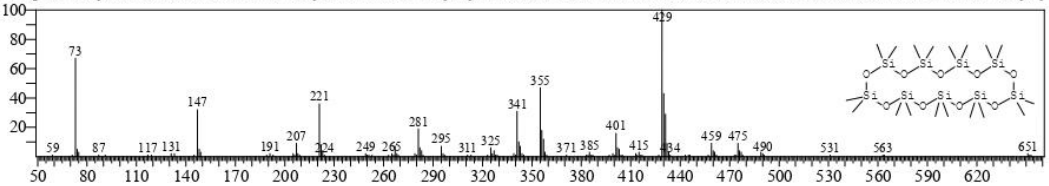
<< Target >>
Line#:57 R.Time:25.515(Scan#:4704) MassPeaks:458
RawMode:Averaged 25.510-25.520(4703-4705) BasePeak:221.10(654231)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



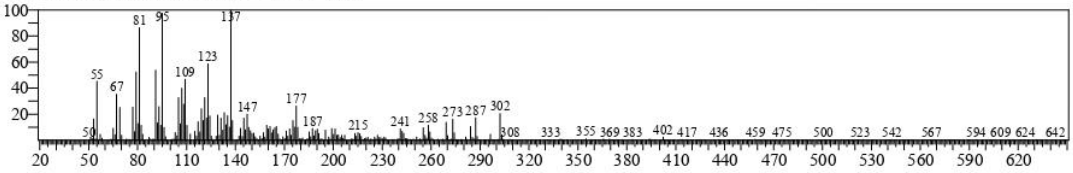
Hit#:1 Entry:39158 Library:NIST17s.lib
SI:74 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



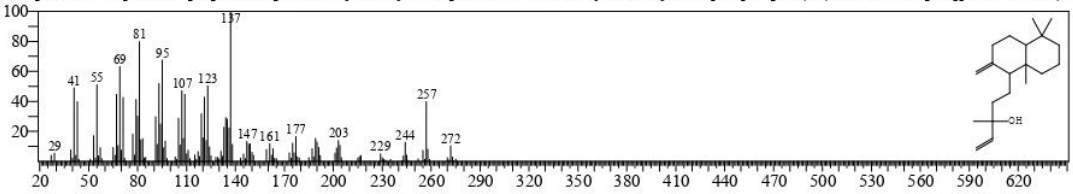
Hit#:2 Entry:39159 Library:NIST17s.lib
SI:68 Formula:C18H54O9Si9 CAS:556-71-8 MolWeight:666 RetIndex:1860
CompName:Cyclononasiloxane, octadecamethyl- $$ Octadeamethyl-cyclononasiloxane $$ 2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18-Octadecamethylcy



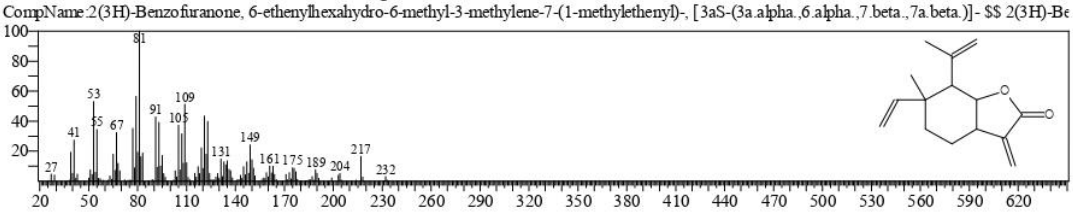
<< Target >>
Line#:58 R.Time:26.190(Scan#:4839) MassPeaks:398
RawMode:Averaged 26.185-26.195(4838-4840) BasePeak:137.15(1121727)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



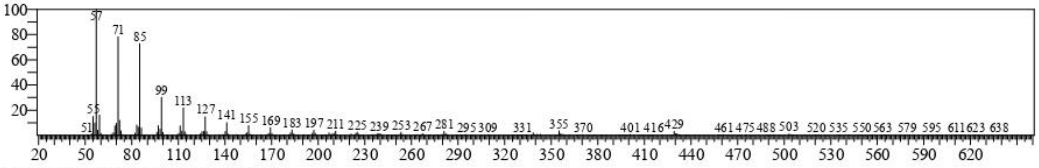
Hit#:1 Entry:32335 Library:NIST17s.lib
SI:78 Formula:C20H34O CAS:1438-62-6 MolWeight:290 RetIndex:2016
CompName:1-Naphthalenepropanol, .alpha.-ethenyldecahydro-.alpha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.(R*),4a.beta.,8a.alpha.]]- $$ Labda-8(2



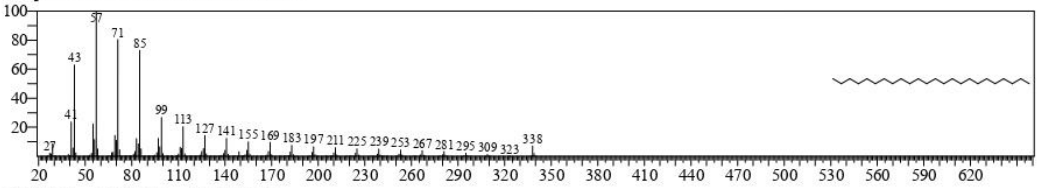
Hit#:2 Entry:26702 Library:NIST17s.lib
SI:75 Formula:C15H20O2 CAS:28290-35-9 MolWeight:232 RetIndex:1725
CompName:2(3H)-Benzofuranone, 6-ethenylhexahydro-6-methyl-3-methylene-7-(1-methylethenyl)-, [3aS-(3a.alpha.,6.alpha.,7.beta.,7a.beta.)]- $$ 2(3H)-Be



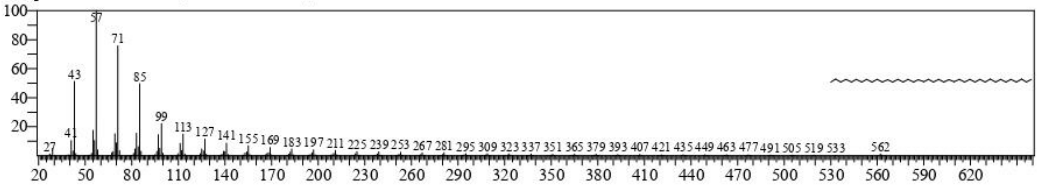
<< Target >>
Line#:59 R.Time:26.275(Scan#:4856) MassPeaks:343
RawMode:Averaged 26.270-26.280(4855-4857) BasePeak:57.10(1804289)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



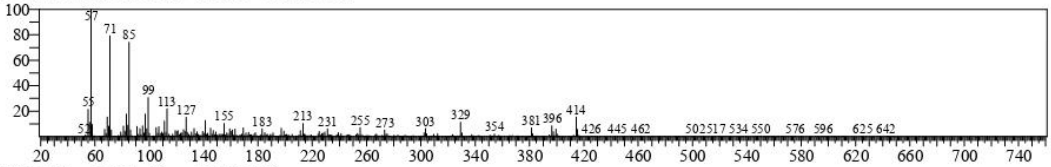
Hit#:1 Entry:35410 Library:NIST17s.lib
SI:91 Formula:C24H50 CAS:646-31-1 MolWeight:338 RetIndex:2407
CompName:Tetracosane $$ n-Tetracosane $$



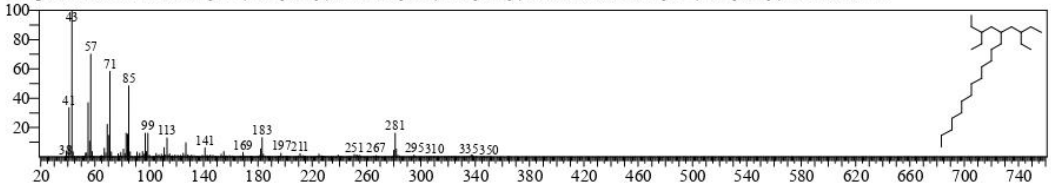
Hit#:2 Entry:38991 Library:NIST17s.lib
SI:90 Formula:C40H82 CAS:4181-95-7 MolWeight:562 RetIndex:3997
CompName:Tetracontane $$ n-Tetracontane $$



<< Target >>
Line#:60 R.Time:26.940(Scan#:4989) MassPeaks:429
RawMode:Averaged 26.935-26.945(4988-4990) BasePeak:57.10(2033084)
BG Mode:Calc. from Peak Group 1 - Event 1 Scan



Hit#:1 Entry:36609 Library:NIST17s.lib
SI:78 Formula:C26H54 CAS:55282-12-7 MolWeight:366 RetIndex:2413
CompName:Octadecane, 3-ethyl-5-(2-ethylbutyl)- $$ 3-Ethyl-5-(2'-ethylbutyl)octadecane $$ 3-Ethyl-5-(2-ethylbutyl)octadecane # $$



Hit#:2 Entry:39209 Library:NIST17s.lib
SI:78 Formula:C54H110 CAS:5856-66-6 MolWeight:758 RetIndex:5389
CompName:Tetrapentacontane