
**UPHLC-MS/MS-GNPS BASED PHOTOCHEMICAL INVESTIGATION OF EUCLEA
RACEMOSA AND ITS ANTIMICROBIAL ACTIVITY**

BY

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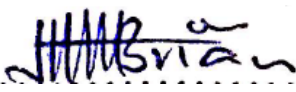
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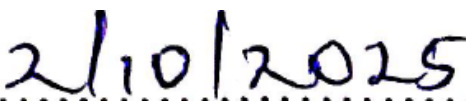
DECLARATION

I understand, declare that this research report is my original work and it has never been submitted to any institution for any academic award except where due reference is made in the text of the thesis.

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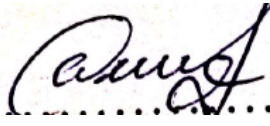
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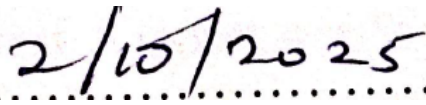
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SUPERVISORS APPROVAL

This research report is submitted as a partial fulfilment for the award of bachelor science and education of Busitema University with approval of the academic supervisor

Supervisor: DR. ANDIMA MOSES

Signature. 

Date. 

DEDICATION

Special thanks dedicated to the almighty God who has seen me through the entire studies right from primary school to university level.

This research report would not have been a success without my beloved father WALUSAGA MOSES, all my siblings and my great friends especially Natabi Manjeri, Makooma Benard, Musisi Pascal, and other coursemates who have always encouraged me that I can make it.

ACKNOWLEDGEMENT

I would like to express my sincere gratitude to all individuals who have supported me and contributed to this research study.

More gratitude is extended to my supervisor Dr. Andima Moses for his guidance, insightful feedback and continuous support through out this research. His expertise and encouragement were valuable in shaping the direction and quality of this work.

ABSTRACT

Euclea racemosa has leathery foliage that can be exceptionally even and dense making it an ideal plant for hedges . A dioecious tree (male and female flower on separate plant). It produces white flowers, which are followed by red, purple and black fruits that attract birds .

Euclea racemosa, commonly known as the “sea guarrie” is a small to medium sized evergreen tree native to the African Indian ocean coast, ranging from Egypt to south Africa. This adaptable plant thrives in diverse habitats like dry woodland, bushland, riverine forests. Due to its growth habit, it is often used as a hedge and is valued locally for its edible fruits, which are sometimes processed into “guarrie vinegar” ailments. Traditionally, *Euclea racemosa* has been utilized in traditional medicine for various ailments. With recent research focusing on its potential laxative properties derived from its root extract .

Basing on Network pharmacology, molecular docking and molecular dynamics simulations studies, A lot of investigations in molecular mechanisms in the management of Dental carries

Potential target genes of *euclea racemosa* were predicted using Swiss target prediction data base. The Gencards, OMIM and DisGeNet databases were used to compile a comprehensive list of genes associated with Dental carries. A compound -disease-network was constructed, and protein- protein interaction networks were analysed to identify hub genes. Finally, molecular docking and interaction of analysis between *euclea racemosa* and the identified proteins were performed using AutoDock tools.

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CHAPTER 1: INTRODUCTION

In the context of Dental caries, network pharmacology can be utilized to identify bioactive compounds from medicinal plants like *Euclea racemosa* that may influence various biological pathways involved in oral health .

1.1 NETWORK PHARMACOLOGY

Network pharmacology is an innovative approach that integrates systems biology with pharmacology to understand the complex interactions between drugs and biological systems . This methodology emphasizes the importance of multiple targets and pathways rather than focusing on a single target, which is typical in traditional

1.2 MOLECULAR DOCKING

Molecular Docking is a computational technique used to predict the preferred orientation of one molecule (typically a drug or ligand) when bound to another molecule (usually a protein) . This method allows researchers to estimate the binding affinity and interaction patterns between potential therapeutic agents derived from *Euclea racemosa* and specific targets related to dental caries. In studying dental caries, Molecular dynamics simulations can help elucidate how bioactive compounds from *Euclea racemosa* affect the stability and conformation of proteins associated with cariogenic bacteria

Dental caries, commonly known as cavities, are a prevalent oral health issue characterized by the decay of tooth structure due to the action of bacterial bacteria which metabolize sugars and starches from food, producing acids that erode the tooth's hard outer layer, known as enamel. . If not addressed promptly, this process can lead to deeper decay, resulting in pain, infection, and potentially tooth loss. The development of dental caries is influenced by various factors including dietary habits, oral hygiene practices among others.

1.3 CLASSIFICATION OF EUCLEA RACEMOSA

1.4 STATEMENT OF THE PROBLEM

There is lack of comprehensive phytochemical investigations on *euclea racemosa* that hinders the development of this plant as potential source of novel antimicrobial agents. Despite its traditional use, phytochemical analysis of *euclea racemosa* has identified various bioactive compounds, including flavonoids, phenolic acids, and terpenoids responsible for its therapeutic effects on dental caries. Therefore, a comprehensive network pharmacology, molecular docking and evaluation of the antimicrobial activity on *euclea racemosa* are highly required.

1.5 OBJECTIVES OF THE STUDY

- To identify the bioactive compounds, and assess the mechanism responsible for the antimicrobial activity of *Euclea racemosa* using network pharmacology

1.6 SIGNIFANCE OF THE STUDY

This research is aimed at elucidating how traditional medicines (euclear racemose) interact with the body to cause curing of dental carries disease. This help to increase the consumption of euclear racemose by patients of dental carries for proper personal hygiene.

CHAPTER 2: LITERATURE REVIEW

2.0 CLASSIFICATION OF EUCLEA RACEMOSA

Euclea racemosa belongs to Ebenaceae family, with the genus name “Euclea” derived from a Greek word meaning “good report”.

They are primarily found along the Indian Ocean coast of Africa, from Egypt to South Africa, also occurring in Comoros.

Euclea racemosa primarily focuses on traditional medicinal uses across various African religions, particularly for treating constipation due to laxative properties, alongside studies exploring its phytochemistry and potential biological activities for its extracts; with research often highlighting its bark and root as the primary parts used in traditional medicine and some literatures mentions its use for skin conditions, stomach ailments, and as an anti-inflammatory agent. The studies on the phytochemistry of *E. racemosa* in evaluation of the vivo laxative effects of aqueous root extracts of *E. racemosa*. This is found that root extract of *E. racemosa* contains secondary metabolites such as saponins, tannins, flavonoids, phenols and terpenes. These metabolites are responsible for the plant’s laxative, stimulant, and GI propulsive activities. The review also found out that plants in the genus *Euclea* contain naphthoquinones, which is used in traditional medicine to treat a variety of conditions including diabetes, toothaches, diarrhea, cancer, malaria, leprosy and HIV/AIDS – related diseases.

2.2 DENTAL DISEASE

Dental disease, also known as oral diseases, are significant global health burden, affecting billions of people worldwide and causing pain, discomfort, and functional limitations. The conditions are largely preventable but can lead to various health issues if left untreated

Common dental diseases include;

Dental caries (tooth decay); is the most common health condition globally affecting nearly adult at some point in their lives.it occurs in bacteria plaque, a sticky film on teeth, convert sugars from food and drink into acids with symptoms toothache, sensitivity to hot, the visible black spots on teeth etc

Periodontal (Gum) diseases; this affects the issues supporting the tissue. The range from gingivitis(this is the earliest and mildest form, characterized by red, swollen and reversible professional cleaning and diligent oral hygiene) to severe periodontitis(this where infections spreads beneath the gums, affecting the bone and ligaments that hold the tooth in place, with symptoms of bad breath, receding gums etc)

2.2.1 BOTANY AND TRADITIONAL USES OF EUCLEA RACEMOSA

Euclea racemosa is characterized as a small to medium-sized evergreen tree. It is part of the Ebenaceae family. Its distribution spans from Egypt to South Africa along the Indian Ocean coast, including Comoros, Oman, and Yemen.

The plant features alternate, opposite to sub-opposite, or pseudo-whorled leaves. It has dioecious inflorescences, meaning it has separate male and female plants.

Traditional Uses

Medicinal:

Toothache and Dental Hygiene: Roots and twigs are used as toothbrushes, and root extracts are applied to the gums and teeth for pain relief and cleaning.

Skin Conditions: Root extracts are used to treat wounds, abscesses, and skin diseases.

Gastrointestinal Issues: Root extracts are used for treating diarrhea, ulcers, and other gastrointestinal disturbances.

Other ailments: *Euclea racemosa* is also traditionally used to treat conditions like cancer, miscarriage, jaundice, snakebites, and gonorrhea.

Antimicrobial Properties: Extracts from *Euclea* species, including *E. racemosa*, are known for their antimicrobial, antifungal, and antioxidant properties, which likely contribute to their medicinal uses.

Other Applications:

Dye: The fruits are used to produce a purple dye for basket fibers and ink.

Fermentation: Fruits are used in the fermentation process for beer production.

Firewood and Timber: The wood is used for firewood and sometimes for tool handles and carving.

Livestock Fodder: Leaves and fruits are used as fodder for livestock.

2.3 TREATMENT OF DENTAL CARIES

There various factors contributing to tooth decay that is to say poor oral hygiene, high sugar diets, acidic beverages and diminished saliva flow. However, treatment of dental diseases varies depending on the specific condition and it's severity.

For tooth decay, early demineralization can some times be reversed with fluoride treatments. Once cavities form, a dental crown may be used to cover and protect the tooth. When decay reaches the tooth's pulp, a root canal procedure is performed to remove the infected pulp and save the tooth.

Gum disease in it's early stage(gingivitis) is reversible with professional dental cleanings and improved oral hygiene. For mild to periodontitis, scaling and root planning(a deep cleaning procedure) removes plaque and tartar from below the gum line.



Figure 1 samples of tooth decay

2.3. TRADITIONAL AND CONVENTIONAL TREATMENT

2.3.1 TRADITIONAL TREATMENT

Traditional treatments for dental caries (tooth decay) historically and currently include restorative procedures like fillings, which remove decay and fill the cavity, while traditional home remedies include using saltwater rinses for pain relief and green tea or clove oil for potential benefits against bacteria and enamel health.

Traditional Home Remedies

Saltwater rinses: A warm saltwater rinse can help relieve pain, reduce bacteria, and clean the area, especially if there is an infection or pus around the tooth.

Clove oil: Historically used for its numbing effect to alleviate pain and its potential to help the tooth retain minerals.

Green tea: Studies suggest that green tea can have antibacterial properties that may help improve oral hygiene and combat plaque and caries, according to the Japan shop oryoki website.

Ginger and chamomile: Ginger has been used for pain relief due to its natural properties, while chamomile can be used in a rinse for its anti-inflammatory benefits, notes Colgate

2.3.2 CONVENTIONAL TREATMENT

Conventional treatment for dental caries, or cavities, primarily involves the total removal of decayed tissue using dental drills, followed by the placement of a filling. This method, also called conventional restoration, is effective but carries a risk of pulp exposure or damage. Newer approaches, such as chemo-mechanical removal, selectively soften and remove decayed tissue, while methods like the Hall-technique involve sealing cavities to arrest decay.

Conventional Treatment Process

Caries Removal: Decayed tooth material is completely removed using rotary instruments.

Restoration: After the decay is cleared, a filling is placed to reconstruct the tooth structure. Common filling materials include dental amalgam and tooth-colored composite resin.

2.4.1 EUCLEA RACEMOSA

Euclea racemosa belongs to Ebenaceae family, with the genus name “*Euclea*” derived from a Greek word meaning “good report”.

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2.4.2 ANTIMICROBIAL ACTIVITY OF EUCLEA RACEMOSA

Euclea racemosa exhibits notable antimicrobial activity, particularly against various bacterial strains, which supports its traditional medicinal uses. The plant's efficacy is attributed to its rich phytochemical profile including flavonoids, glycosides, phenols, saponins and triterpenes. Studies have been shown that *Euclea racemosa* extracts, especially those prepared with methanol, demonstrate significant antibacterial effects which are effective against both Gram-positive and Gram-negative including *staphylococcus aureus*, *streptococcus pneumoniae*, *streptococcus pyogenes*.

CHAPTER 3: MATERIALS AND METHODS

Data mining from web repositories such as google scholar, PubChem, Swiss prediction were used to search and identify the bioactive compounds from Euclea racemosa, the phyto-constituents specifically in euclea racemosa were being used.

Prediction of target genes of euclea racemosa

The possible human target genes of euclea racemosa were identified using Swiss target predict. To obtain the swiss target genes, the search included genes for organisms basically Homo sapiens to ensure relevance to human biology. The duplicated genes were eliminated using Microsoft Excel to arrive at final target gene list.

Prediction target genes for dental caries

The human target genes associated with dental caries were obtained from online Databases including Gene cards, DisGeNET and the online Mendelian in Man (OMIM). The key word was dental caries in humans which excuted the search and the duplicated genes were removed in order to arrive to the complete list of genes for dental caries.

Protein interaction (PPI) Network construction and analysis Protein-

The STRING database version 12 (link) was used to construct to PPI network of euclea racemosa and the genes of dental caries, limiting the analysis to human proteins, with High confidence interactions ([confidence score \$\geq 10\$](#)) which should be used to select nodes for network visualization, that facilitates the creation of reliable PPI network, that the interactions are highly reliable, biologically relevant, derived from high quality data.

Gene ontology and Kyoto encyclopedia of genes and genomes (KEGG) enrichment studies

This further understands the different biological mechanisms underlying the potential activity of euclea racemosa, gene ontology(GO) and Kyoto encyclopedia of Gene and Genomes(KEGG) pathway enrichment analysis on the compound target disease network were performed using the Database for Annotation, visualization and Inter-grated Discovery(DAVID)

Drug-likeness prediction and toxicity screening of euclea racemosa

Euclea racemosa, a plant used traditionally for various ailments, has shown promising results in drug-like prediction and toxicity screening. Studies indicate it is generally safe, with an LD50 (lethal dose for 50% of subjects) greater than 2000 mg/kg. The plant's extracts, particularly from the root, exhibit laxative effects in mice and have shown antimicrobial properties. Further research into its phytochemical composition and biological activity could lead to the development of new drugs.

Drug-like Prediction and Toxicity Screening:

Phytochemical Screening:

Euclea racemosa contains various bioactive compounds, including naphthoquinones, terpenes, saponin, flavonoids, lignins and phones

Toxicity Studies: Acute toxicity studies, following OECD guidelines, have shown that *E. racemosa* is safe at high doses (e.g., 2000 mg/kg) with no observed deaths or toxic signs. Sub-acute toxicity studies (e.g., 28 days) have also shown no adverse effects.

Laxative Effects: Aqueous root extracts of *E. racemosa* have demonstrated laxative properties in mice, increasing fecal water content and affecting gastrointestinal transit.

Antimicrobial Activity: *E. racemosa* extracts, especially from the root, have shown antibacterial activity against certain bacteria.

Potential for Drug Development: The presence of bioactive compounds and the demonstrated pharmacological properties (antimicrobial, laxative, etc.) suggest potential for developing new drugs from *E. racemosa*.

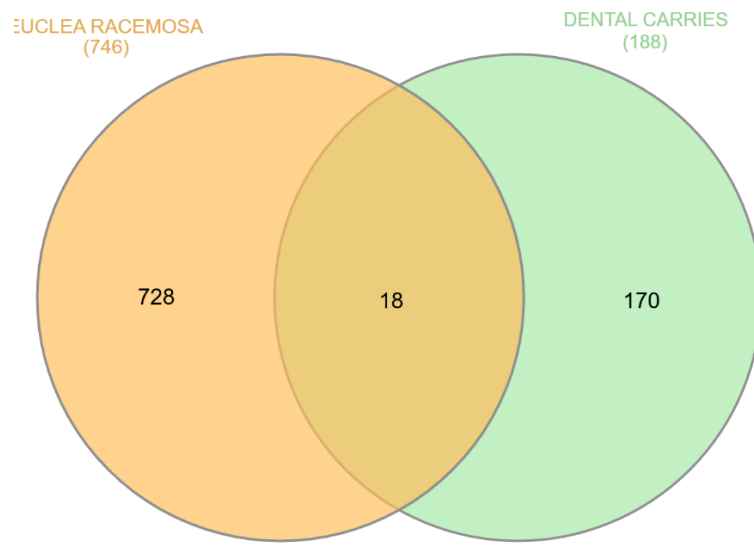
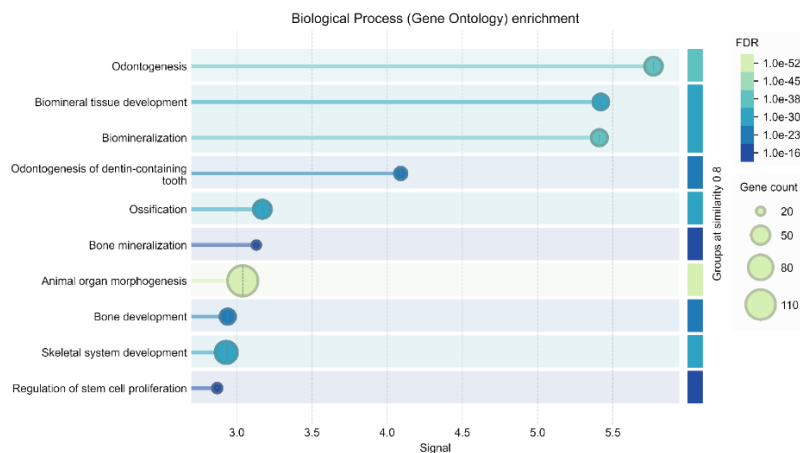
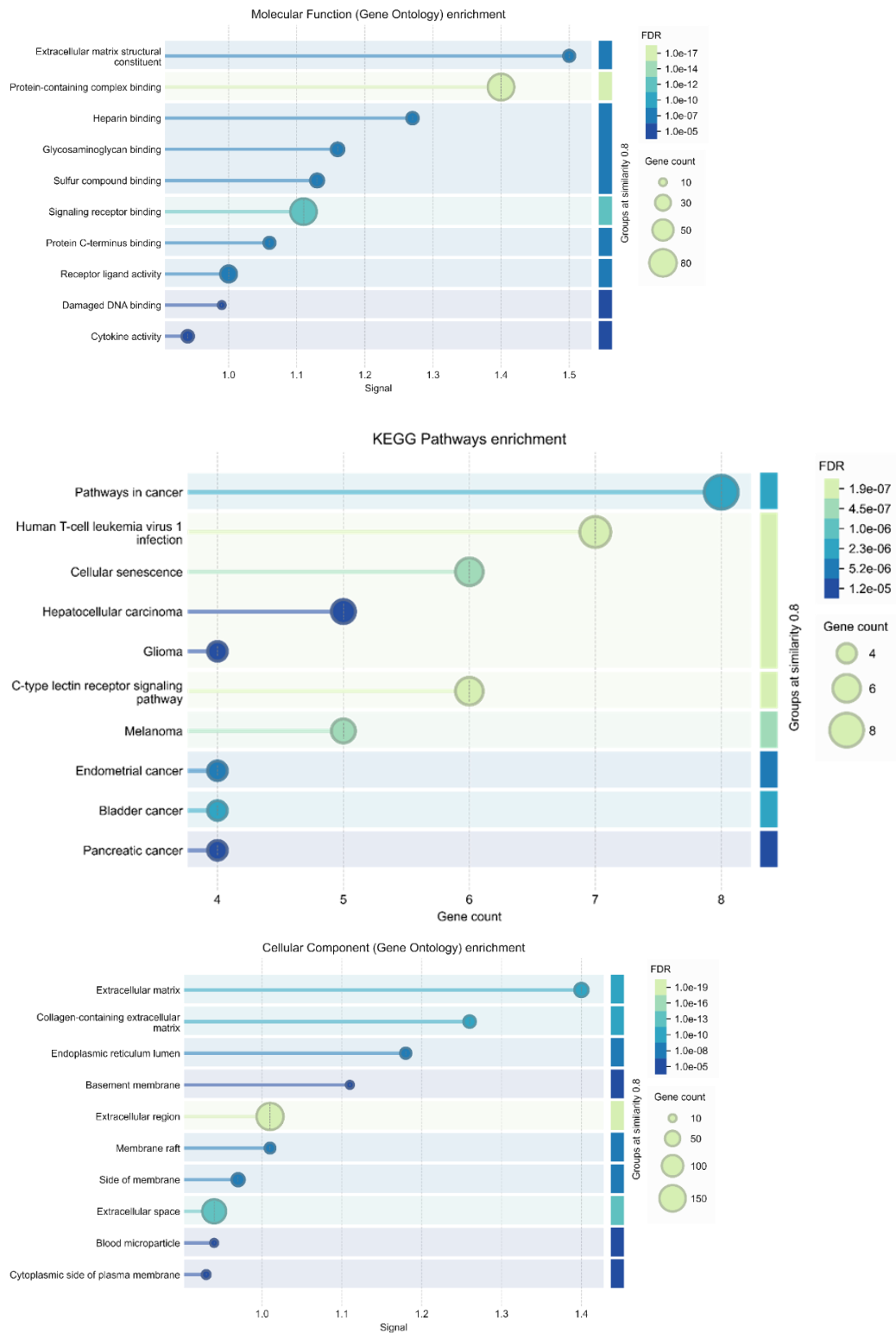


Figure 3: a venn diagram showing potential targets of *euclea racemosa* and *streptococcus mutans* dental caries

The genes in the intersection were;

PTGFR, PTGER3, CTSK, CTSS, PTGS2, MDM4, FAAH, PLA2G2A, ALPL, SLC2A1, ADORA1, CYP1B1, F3, LCK, CPT2, ECE1, XDH, PIK3CD





Network pharmacology-based analysis. Prediction of potential targets of compounds and collection of targets for HPLC-MS

PPI network analysis. The PPI network reveals the potential connection between targets. After removing the free genes. The protein targets identified in the protein Data Bank (PDB), along with their respective PDB ID's, and resolution

4.2 MOLECULAR DOCKING

The autodock tools software version 1.5.7 was used to analyse the intersections between the AE and the identified hub genes. The 3-dimensional structures of the target genes IL6,TNF,IL1B were obtained from protein Data bank as PDB formats. These were prepared for binding by adding polar hydrogens,eliminating water molecules, and removing residual chains and ligands.

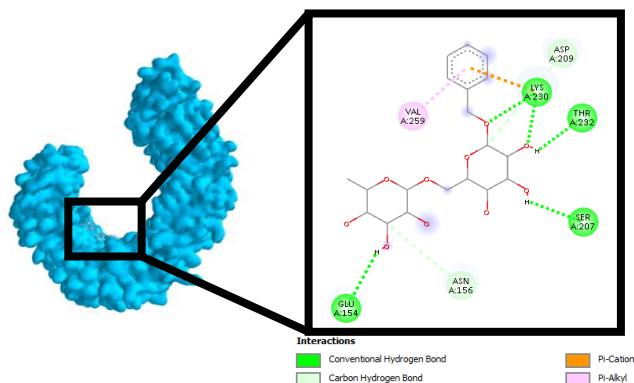


Figure 4: Molecular docking results

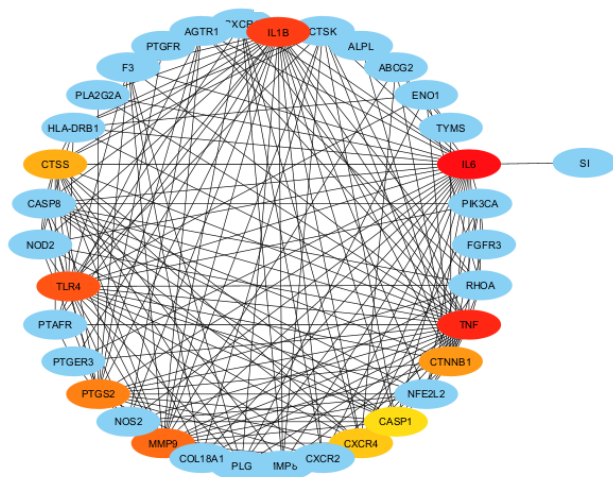


Figure 5: Cytohubba herb genes disease-compound target network interaction streptococcus dental caries

The network contained 35 nodes with an average node degree of 10. The size and color of the node reflects the importance of the degree. The larger the degree, the more important the node is in the network, suggesting it may be a key target in HPLC-MS treatment. To make the figure clear, we used diamond to highlight the top 10 genes in all the nodes. According to the degree value, the top 10 were regarded as hub genes as shown in the table below

Top 10 in networking interactions		
RANK	NAME	SCORES
1	IL6	28
2	TNF	26
3	IL1B	25
4	TLR4	23
5	MMP9	22
6	PTGS2	21
7	CTNNB1	17
8	CTSS	16
9	CXCR4	15
10	CASP1	14

IL6- interleukin 6; is an interleukin that acts as both a pro inflammatory cytokines and an anti-inflammatory myokine. This cytokine is a type of a protein that plays a role in the immune system with a composition of 184-212 amino acids for development of antigen-specific immune responses by promoting the differentiation of Th2 and Th17 cells

TNF-Tumor Necrosis factor; is a cytokine, a signaling molecule produced by the immune system, primarily by activated macrophages for triggering inflammations which is the body's initial response to injury and infections.

RECOMMENDATIONS

One objective has not been achieved for example reducing on dental caries infection by use of euclea racemose from the environment since it required synthesis of a specific drug.

This calls for further studies on molecular mechanism of bioactive compounds from euclea racemose to find out their anti-dental activity since targets and genes associated to dental caries infections have been identified.

APPENDIX

The table below relates the different compounds with their retention time

#	RT(Min)	precursor	Adduct ion	Molecular Formula	Exact Mass	Compound Annotation
1	11.97	177.164	M+H	C ₁₃ H ₂₂ O	194.167	2-Butanone, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
2	1.93	181.049	M+H-H ₂ O	C ₉ H ₁₀ O ₅	198.053	4-Hydroxy-3,5-dimethoxy-benzoic acid
3	12.7	191.179	M+H-H ₂ O	C ₁₄ H ₂₆ O ₂	226.193	2,4,7,9-Tetramethyl-dec-5yne-4,7-diol
4	1.21	291.086	M+H	C ₁₅ H ₁₄ O ₆	290.079	2-(3,4-Dihydroxy-phenyl) chroman-3,5,7-triol
5	7.08	197.129	M+H	C ₁₀ H ₁₆ N ₂ O ₂	196.121	3-Isopropyl-hexahydro-pyrrolo[1,2- α] pyrazine 1,4-dione
6	9.27	786.6	M+H	C ₄₄ H ₈₄ NO ₈ P	785.594	1-Stearoyl-2-linoleoyl-sn-glycero-3-phosphocholine
7	8.52	496.34	M+H	C ₂₄ H ₅₀ NO ₇ P	495.33	Lyso-pc(16:0)
8	0.51	220.118	M+H	C ₉ H ₁₉ NO ₅	219.11	3-(2,4-dihydroxy-3,3-dimethylbutyramino) propanoic acid
9	7.49	445.212	M+H	C ₂₇ H ₂₈ N ₂ O ₄	444.20	Aurantiamide acetate Asperglaucide, Lyciumamide 6.N-Benzoylphenylalanylphenylalinal acetate
10	6.61	288.253	M+H	C ₁₆ H ₃₃ NO ₃	287.25	Lauryl diethanolamide
11	7.84	391.284	M+H	C ₂₄ H ₃₈ O ₄	390.28	BIS(2-ETHYLHEXYL)PHTHALATE
12	7.22	319.097	M+H	C ₂₀ H ₁₄ O ₄	318.09	3,3-Bis(4-hydroxy-phenyl)-3H-isobenzofuran-1-one
13	9.53	403.233	M+H	C ₂₀ H ₃₄ O ₈	402.48	3-Acetoxy-3-butoxycarbonylpentanedioic acid dibutyl ester
14	10.23	772.586	M+H	C ₄₄ H ₈₆ NO ₇ P	771.614	1-(1Z-Octadecenyl)-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
15	10.33	778.54	M+H	C ₄₄ H ₇₆ NO ₈ P	777.531	1,2-Di-(9Z,12Z,15Z-octadecatrienoyl)-sn-glycero-3-phosphocholine

16	8.04	782.568	M+Na	C ₄₂ H ₈₂ NO ₈ P	759.578	1-Hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
17	9.46	760.586	M+H	C ₄₂ H ₈₂ NO ₈ P	759.578	1-Hexadecanoyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
18	4.42	273.08	(M+H)+	C ₁₅ H ₁₂ O ₅	272.068	5,7-dihydroxy-2-(4-hydroxyphenyl)-2,3-dihydro-4H-chromen-4-one
19	1.26	579.15	M+H	C ₃₀ H ₂₆ O ₁₂	578.142	Procyanidin B2
20	7.08	197.129	M+H	C ₁₀ H ₁₆ N ₂ O ₂	196.12	Isopropyl-hexahydro-pyrrole(1,2- α) pyrazine-1,4-dione
21	7.75	306.104	M+h	C ₁₁ H ₂₀ N ₃ O ₃ PS	305.10	2-[[tert-butoxy)carbonyl]amino}-3-[4-(difluoromethyl)phenyl]propanoic acid 3-[4-(difluoromethyl)phenyl]-2-[(2-methylpropan-2-yl)oxycarbonylamino]propanoic acid
22	9.46	300.289	M+H	C ₁₈ H ₃₇ NO ₂	299.282	Hexadecanoicacid (2-hydroxyethyl)-amide
23	9.81	201.164	M-2H ₂ O+H	C ₁₅ H ₂₄ O ₂	236.178	1-(1,5-Dimethyl-hex-4-enyl)-4-methyl-2,3-dioxabicyclo(2.2.2)Oct-5-ene
24	7.43	318.3	M+H	C ₁₈ H ₃₉ NO ₃	317.293	2-Amino-octadecane-1,3,4-tiol
25	9.51	311.258		C ₁₉ H ₃₆ O ₄	328.261	1,4-dihydroxyheptadec-16-en-2-yl acetate
26	8.34	279.232	M+H-H ₂ O	C ₁₈ H ₃₂ O ₃	296.235	8-(3-Oct-2-enyl-Oxiranyl)-Octanoic acid
27	1.22	496.202	(M+NH ₄)+	C ₂₀ H ₃₀ O ₁₃	478.17	(2R,3S,4S,5R,6S)-2-[[[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl) oxolan-2-yl]oxymethyl]-6-(3,4,5-trimethoxyphenoxy)oxane-3,4,5-triol
28	7.51	211.144	M+H	C ₁₁ H ₁₈ N ₂ O ₂	210.14	3-Isobutyl-hexahydro-pyrrolo(1,2- α) pyrazine-1,4-dione
29	10.22	255.232	M+H	C ₁₆ H ₃₀ O ₂	254.22	Hexadec-9-enoic acid

30	10.36	237.221	M+H-H ₂ O	C ₁₆ H ₃₀ O ₂	254.225	Hexadec-9-enoic acid
31	9.97	746.569	M+H	C ₄₆ H ₈₄ NO ₇ P	745.599	1-Hexadecyl-2-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine
32	2.9	744.306	(M+NH ₄) ⁺	C ₃₄ H ₄₆ O ₁₇	726.27	
33	0.73	307.082	M+H	C ₁₅ H ₁₄ O ₇	306.07	2-(3,4,5-Trihydro-phenyl-chroman-3,5,7-triol
34	10.04	580.426	M+H	C ₃₀ H ₆₂ NO ₇ P	579.43	1-Behenoyl-2-hydroxy-sn-glycero-3-phosphocholine
35	0.45	325.113	M+H-H ₂ O	C ₁₂ H ₂₂ O ₁₁	342.12	Sucrose
36	7.38	275.201	M+H-H ₂ O	C ₁₈ H ₂₈ O ₃	292.20	9-Oxo-Octadeca-10,12,15-Trienoic acid
37	9.78	282.279	M+H	C ₁₈ H ₃₅ NO	281.27	Octadec-9-enoic acid amide
38	11.97	177.164	M+H-H ₂ O	C ₁₃ H ₂₂ O	194.17	4-(2,6,6-Trimethyl-cyclohex-2-enyl)-butan-2-one
39	2.78	611.16	M+H	C ₂₇ H ₃₀ O ₁₆	610.15	Rutin
40	3.91	207.065	M+H-H ₂ O	C ₁₁ H ₁₂ O ₅	224.07	hydroxycinnamic acid
41	6.34	257.081	M+H	C ₁₅ H ₁₂ O ₄	256.07	Pinocembrin
42	9.86	468.39	M+Na	C ₂₈ H ₅₁ N ₃ O	445.403	Tricos-4-enoic acid [2-(1H-imidazol-2-yl)-ethyl] amide
43	3.03	345.17	M-H ₂ O+H	C ₂₀ H ₂₆ O ₆	362.17	2,3-bis[(4-hydroxy-3-methoxyphenyl) methyl]butane-1,4-diol
44	9.62	307.263	M-H ₂ O+H	C ₂₀ H ₃₆ O ₃	324.66	15-Hydroxy-icosa-11,13-dienoic acid
45	9.34	363.31	M+H	C ₂₀ H ₄₂ O ₅	362.30	2-(2-[2-Decacyclo)-ethoxy]-ethoxy) – ethanol
46	2.15	448.218	M+NH ₄	C ₂₀ H ₃₀ O ₁₀	430.184	2-Phenylethyl 6-O-(6-deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranoside
47	10.42	338.342	M+H	C ₂₂ H ₄₃ NO	334.335	Docos-13-enoic acid amide
48	1.79	600.265	M+NH ₄	C ₂₈ H ₃₈ O ₁₃	582.23	[[5-(4-hydroxy-3,5-dimethoxyphenyl)-6,7-bis(hydroxymethyl)-1,3-dimethoxy-5,6,7,8-tetrahydronaphthalen-2-yl]oxy]-

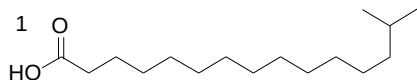
						6-(hydroxymethyl)oxane-3,4,5-triol
49	11.22	329.27	[M+H] ⁺	C ₂₂ H ₄₄ O ₆	404.31	1,2-dihydroxyheptadec-16-en-4-yl acetate
50	6.05	343.29	M	C ₁₉ H ₃₉ N ₂ O ₃ ⁺	343.30	Carboxymethy-(3-dodecanoylamino-propyl)-dimethyl ammonium
51	3.04	391.1	[m+h] ⁺	C ₂₁ H ₂₀ Cl ₂ O ₃	390.08	2-carboxymethyl-2-hydroxyhexyl-trimetylazanium
52	6.2	403.202	M+H	C ₂₅ H ₂₆ N ₂ O ₃	402.19	N-[1-(-Hydromethyl-2-phenylethylcarbamoyl)-2-phenylethyl]-benzamide
53	8.93	281.24	[M+H] ⁺	C ₁₈ H ₃₆ O ₂	280.24	Octadeca-9,12-dienoic acid
54	8.73	480.309	M+H	C ₂₃ H ₄₆ NO ₇ P	479.30	Octadec-9-enoic acid 3-[(2-amino-ethoxy)-hydrophosphoryloxy] -2-hydroxypropyl ester
55	12.4	239.237	M-H ₂ O+H	C ₁₆ H ₃₂ O ₂	256.24	Hexadecanoic acid
56	10.25	718.538	M+H	C ₃₉ H ₇₆ NO ₈ P	717.531	Octadec-9-enoic acid 1-[(2-amino ethoxy)-hydroxyphosphoryloxmethyl]-2-hexadecanoyloxy-ethyl-ester
57	10.37	371.316	M+H	C ₂₂ H ₄₂ O ₄	370.308	Hexanedioic acid bis(2-ethylhexyl) ester
58	9.88	251.047	M+H	C ₁₂ H ₁₁ O ₄ P	250.04	Phosphoric acid diphenyl ester
59	9.53	425.378	M+h-h ₂ o	C ₃₀ H ₅₀ O ₂	442.38	3a-Hydroxymethyl-1-isopropenyl-5a,5b,8,8,11a-pentamethyl-icosahydrocyclopenta[α]chrysene-9-ol
60	7.54	302.308	M+H	C ₁₈ H ₃₉ NO ₂	301.30	2-Amino-octadecane-1,3-diol
61	7.39	315.253	M+H	C ₁₈ H ₃₄ O ₄	314.25	9,10-Dihydroxy-12Z-octadecenoic acid
62	9.97	439.357	M+H-H ₂ O	C ₃₀ H ₄₈ O ₃	456.36	Oleanic acid
63	2.98	235.06	[M+H] ⁺	C ₁₂ H ₁₀ O ₅	234.05	Anhydrobrazilic Acid
64	1.37	479.176	M+H	C ₂₀ H ₃₀ O ₁₃	478.169	(2R,3S,4S,5R,6S)-2-[(3,4,5-trihydroxyoxan-2-yl)oxymethyl]-6-(3,4,5-trimethoxyphenoxy)oxane-3,4,5-triol

65	8.8	297.242	[M+H ₂ O+H] ⁺	C ₁₈ H ₃₄ O ₄	314.246	8-Hydroxy-8-(3-Octayloxiranyl) octanoic acid
66	9.95	637.305	M+Na	C ₂₃ H ₄₆ N ₆ O ₁₃	614.31	2-Methyl-4-oxo-4H-pyran-3-yl 6-O-(4-carboxy-3-hydroxy-3-methylbutanoyl)-beta-D-glucopyranoside
67	1.42	455.116	M+Na	C ₁₈ H ₃₄ O ₂	432.127	3-Hydroxy-3-methyl-pentanedioic acid mono-[3,4,5-trihydroxy-6-(2-methyl-4-oxo-4H-pyran-3-yloxy)-tetrahydropyran-2-ylmethyl] ester
68	7.72	518.324	M+H	C ₂₆ H ₄₈ NO ₇ P	517.32	2-carboxymethyl-2-hydroxethyl-trimethylazanium.
69	7.4	293.211	M+H-H ₂ O	C ₁₈ H ₃₀ O ₄	310.214	9-Hydroperoxy-octadeca-10,12,15-trienoic acid
70	13.23	203.179	M-H ₂ O+H	C ₁₈ H ₃₀ O ₄	220.183	9-Hydroperoxy-octadeca-10,12,15-trienoic acid
71	7.49	261.123	M+H	C ₁₄ H ₁₆ N ₂ O ₃	260.116	3-(4-Hydroxy-benzyl)-hexahydro-pyrrolo[1,2- α]pyrazine-1,4-dione
72	13.21	429.336	[M+h] ⁺	C ₂₈ H ₄₄ O ₃	428.33	(1S,2R,5R,6R,10R,13S,15S)-5-[(2R,3E,5R)-5,6-dimethylhept-3-en-2-yl]-6,10-dimethyl-16,17-dioxapentacyclo
73	8.93	399.25	M+H	C ₁₈ H ₃₉ O ₇ P	398.24	Phosphoric acid tri-(2-butoxyethyl) ester
74	1.05	450.197	M+NH ₄	C ₁₉ H ₂₈ O ₁₁	432.163	Benzyl 6-O-beta-D-glucopyranosyl-beta-D-glucopyranoside
75	6.51	371.099	M+Na	C ₂₀ H ₁₆ N ₂ O ₄	348.111	4-Ethyl—4-hydro-1,12-dihydro-4H,2-oxa-6,12a-diazadibenzo[b,h]fluorene-3,13-dione
76	2.5	289.071	M+H	C ₁₅ H ₁₂ O ₆	288.063	3,5,7-Trihydroxy-2-(4hydroxy-phenyl)-chroman-4-one
77	9.6	461.399	M-H ₂ O+H	C ₃₀ H ₅₄ O ₄	478.402	2,6,10,15,19,23-Hexamethyl-tetracos-6,10,14,18-tetrane-2,3,22,33-tetraol
78	1.3	195.088	[M+H] ⁺	C ₈ H ₁₀ N ₄ O ₂	194.08	Caffein
79	13.19	324.29	M+H	C ₂₀ H ₃₇ NO ₂	323.282	Octadeca-9,12-dienoic acid (2-hydroxy-ethyl)-amide
80	1.77	434.202	M+NH ₄	C ₁₉ H ₂₈ O ₁₀	416.168	Benzyl 6-O-(6-deoxy-alpha-L-mannopyranosyl)-beta-D-glucopyranoside
81	3.1	598.25	M+NH ₄	C ₂₈ H ₃₆ O ₁₃	580.216	2-(4-(4-Hydroxy-3,5-dimethoxy-phenyl)-tetrahydro-

						furo[3,4-C]furan-1-yl-] -2,6-dimethoxy-phenoxy)-6-hydromethy-tetrahydro-pyran-3,4,5-triol
8 2	12.7	191.17 9	M+H- 2H ₂ O	C ₁₄ H ₂₆ O ₂	226.19 3	2,4,7,9-Tetramethyl-dec-5-yne-4,7-diol
8 3	8.22	351.25 3	[M+Na] ⁺	C ₁₉ H ₃₆ O ₄	328.26	Acetic acid-1-(2,3-dihydroxyl-propyl) – tetradic-13-enyl-ester
8 4	9.85	355.28 4	[m+h] ⁺	C ₂₁ H ₃₈ O ₄	354.28	Octadeca-9,12-dienoic acid-2,3-dihydroxy-propyl ester
8 5	1.93	181.04 9	M+H-H ₂ O	C ₉ H ₁₀ O ₅	198.05 3	4-Hydroxy-3,5-dimethyl-benzoic acid
8 6	1.14	480.20 8	M+NH ₄	C ₂₀ H ₃₀ O ₁₂	462.17 4	Hexopyranoside, 3,4-dimethoxyphenyl 6-O-(6-deoxy-alpha-L-mannopyranosyl)-
8 7	4.43	549.30 6	M+H	C ₃₀ H ₄₄ O ₉	548.30	3-(3,5-dihydroxy-4-methoxy-6-methyl-tetrahydroxy-pyran-2-yloxy)-14-hydroxy-13-methyl-17-(5-oxo-2,5-dihydro-furan-3-yl) -hexadecahydro-cyclopenta[α] phenanthrene-10-carbaldehyde
8 8	8.5	293.21 1	M+H-H ₂ O	C ₁₈ H ₃₀ O ₄	310.21 4	9-Oxo-11-(3-pentyl-oxiranyl)-undec-10-enoic acid
8 9	8.26	532.34 8	M+NH ₄	C ₂₇ H ₄₆ O ₉	514.31 4	Octadeca-9,12,15-trienoic acid 2-hydro-3-(3,4,5-trihydroxy-6-hydroxymethyl-tetrahydro-pyran-2-yloxy)-propyl ester

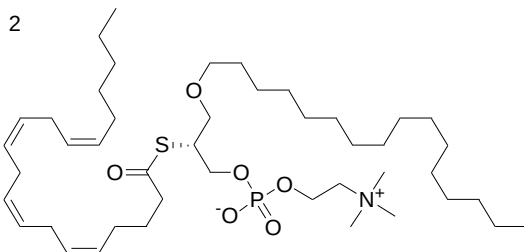
Phytosphingosine

[(2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl) oxolan-2-yl] oxymethyl]-6-(3,4,5-trimethoxyphenoxy) oxane-3,4,5-triol

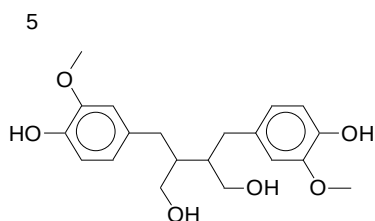


14-Methyl-pentadecanoic acid

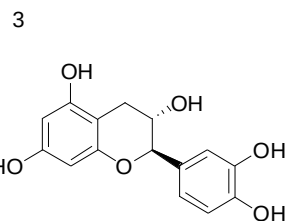
$C_{16}H_{32}O_2$
Exact Mass: 256.24
Mol. Wt.: 256.42
m/e: 256.24 (100.0%), 257.24 (17.9%), 258.25 (1.6%)
C, 74.94; H, 12.58; O, 12.48



$C_{44}H_{82}NO_6PS$
Exact Mass: 783.56
Mol. Wt.: 784.16
m/e: 783.56 (100.0%), 784.56 (50.3%), 785.57 (12.4%), 785.56 (6.2%), 786.57 (2.7%), 786.56 (2.3%), 784.57 (1.2%)
C, 67.39; H, 10.54; N, 1.79; O, 12.24; P, 3.95; S, 4.09

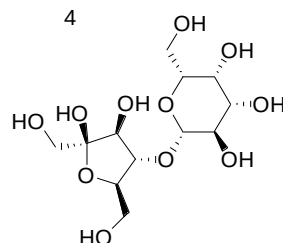


$C_{20}H_{26}O_6$
Exact Mass: 362.17
Mol. Wt.: 362.42
m/e: 362.17 (100.0%), 363.18 (22.9%), 364.18 (3.7%)
C, 66.28; H, 7.23; O, 26.49



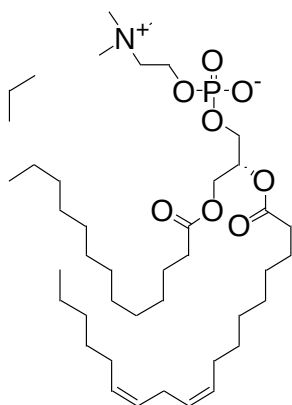
2-(3,4-Dihydroxy-phenyl)-chroman-3,5,7-triol

$C_{15}H_{14}O_6$
Exact Mass: 290.08
Mol. Wt.: 290.27
m/e:
C, 62.07; H, 4.86; O, 33.07

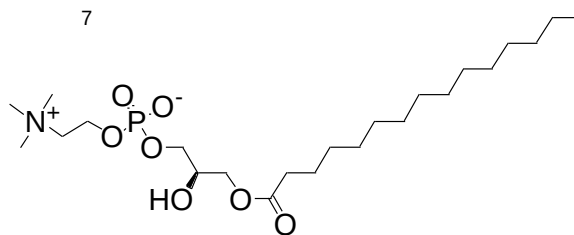


2-(4,5-Dihydroxy-2,5-bis-hydroxymethyl-tetrahydro-furan-3-yloxy)-6-hydroxymethyl-tetrahydro-pyran-3,4,5-triol

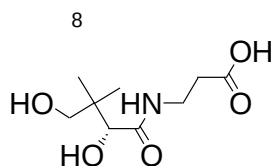
$C_{12}H_{22}O_{11}$
Exact Mass: 342.12
Mol. Wt.: 342.30
m/e: 342.12 (100.0%), 343.12 (14.1%), 344.12 (3.1%)
C, 42.11; H, 6.48; O, 51.42



$C_{44}H_{84}NO_8P$
 Exact Mass: 785.59
 Mol. Wt.: 786.11
 m/e: 785.59 (100.0%), 786.60 (50.5%), 787.60 (14.1%), 788.60 (2.7%)
 C, 67.23; H, 10.77; N, 1.78; O, 16.28; P, 3.94

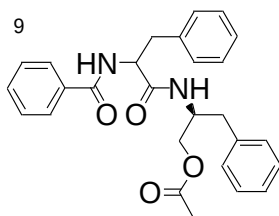


7
 $C_{23}H_{47}NO_7P$
 Exact Mass: 480.31
 Mol. Wt.: 480.60
 m/e: 480.31 (100.0%), 481.31 (26.2%), 482.32 (3.4%), 482.31 (1.5%)
 C, 57.48; H, 9.86; N, 2.91; O, 23.30; P, 6.44



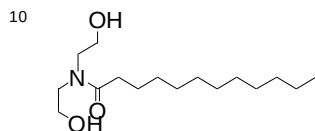
8
 3-(2,4-Dihydroxy-3,3-dimethyl-butylamino)-propionic acid

$C_9H_{17}NO_5$
 Exact Mass: 219.11
 Mol. Wt.: 219.23
 m/e:
 C, 49.31; H, 7.82; N, 6.39; O, 36.49



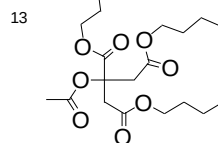
9
 Acetic acid 2-(2-benzoylamino-3-phenyl-propionylamino)-3-phenyl-propyl ester

$C_{27}H_{28}N_2O_4$
 Exact Mass: 444.20
 Mol. Wt.: 444.52
 m/e: 444.20 (100.0%), 445.21 (30.6%), 446.21 (5.5%)
 C, 72.95; H, 6.35; N, 6.30; O, 14.40



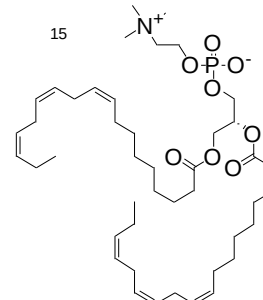
Dodecanoic acid bis-(2-hydroxy-ethyl)-amide

$C_{16}H_{33}NO_3$
Exact Mass: 287.25
Mol. Wt.: 287.44
m/e: 287.25 (100.0%), 288.25 (18.4%), 289.25 (2.2%)
C, 66.86; H, 11.57; N, 4.87; O, 16.70

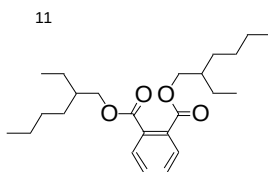


3-Acetoxy-3-butoxycarbonyl-pentanedioic acid dibutyl ester

$C_{20}H_{34}O_8$
Exact Mass: 402.23
Mol. Wt.: 402.48
m/e: 402.23 (100.0%), 403.23 (23.1%), 404.23 (4.1%)
C, 59.68; H, 8.51; O, 31.80

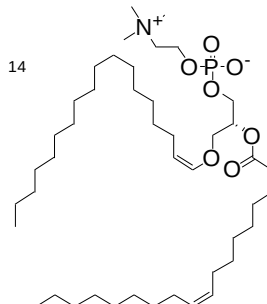


$C_{44}H_{76}NO_8P$
Exact Mass: 777.53
Mol. Wt.: 778.05
m/e: 777.53 (100.0%), 778.53 (49.3%), 779.54 (14.0%), 780.54 (2.8%), 778.54 (1.5%)
C, 67.92; H, 9.85; N, 1.80; O, 16.45; P, 3.98

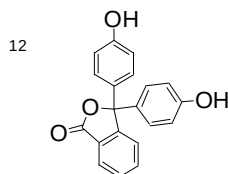


Phthalic acid bis-(2-ethyl-hexyl) ester

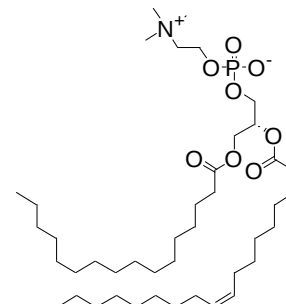
$C_{24}H_{38}O_4$
Exact Mass: 390.28
Mol. Wt.: 390.56
m/e: 390.28 (100.0%), 391.28 (27.4%), 392.28 (4.3%)
C, 73.81; H, 9.81; O, 16.39



$C_{44}H_{76}NO_8P$
Exact Mass: 771.61
Mol. Wt.: 772.13
m/e: 771.61 (100.0%), 772.62 (50.5%), 773.62 (13.9%), 774.62 (2.6%)
C, 68.44; H, 11.23; N, 1.81; O, 14.50; P, 4.01

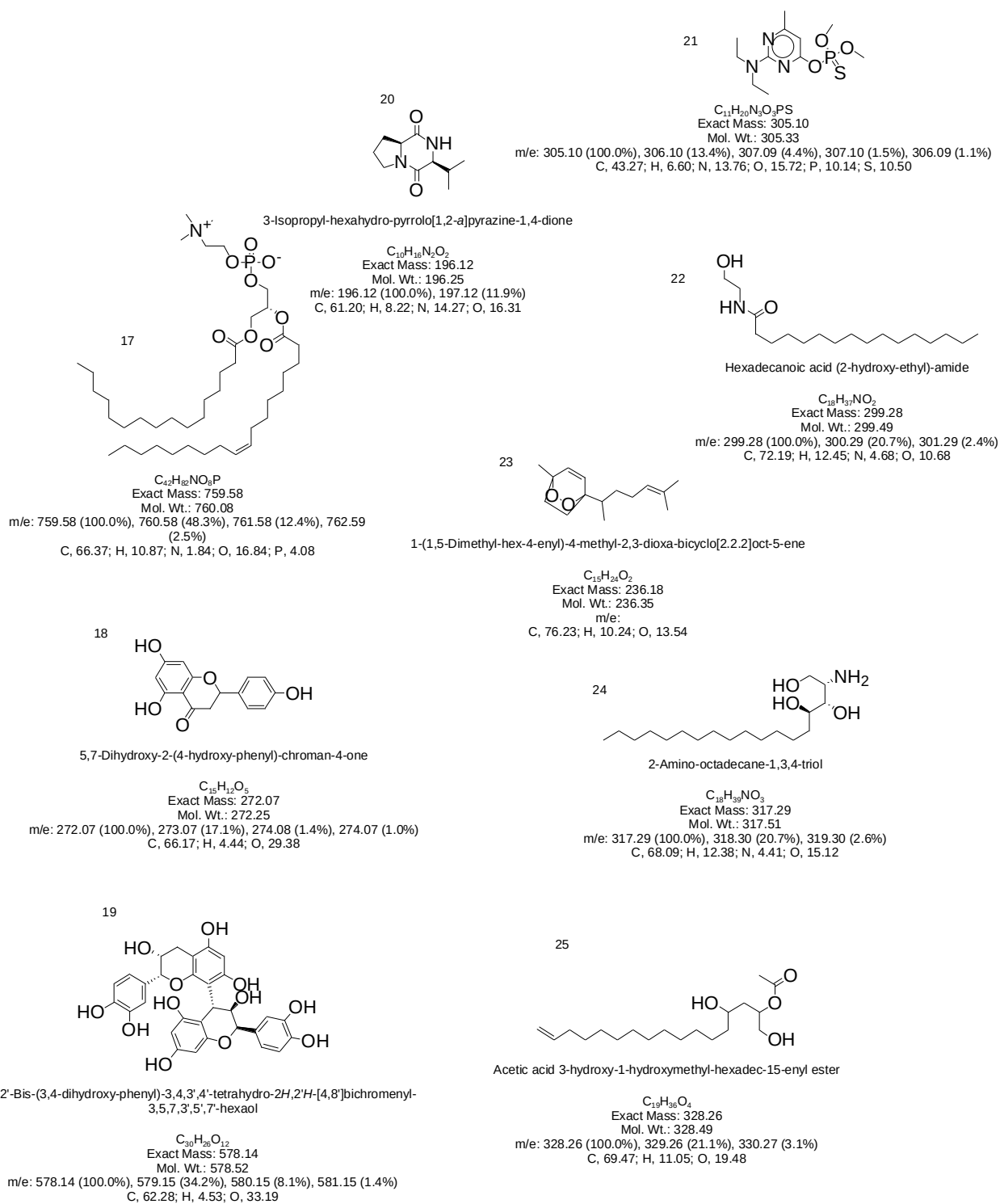


3,3-Bis-(4-hydroxy-phenyl)-2H-isobenzofuran-1-one
Exact Mass: 318.09
Mol. Wt.: 318.32
m/e: 318.09 (100.0%), 319.09 (22.4%), 320.10 (2.4%)
C, 75.46; H, 4.43; O, 20.10

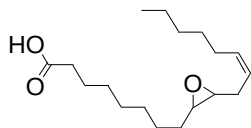


$C_{42}H_{82}NO_8P$
Exact Mass: 759.58
Mol. Wt.: 760.08
m/e: 759.58 (100.0%), 760.58 (48.3%), 761.58 (12.4%), 762.59 (2.5%)
C, 66.37; H, 10.87; N, 1.84; O, 16.84; P, 4.08

S



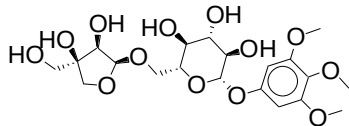
26



8-(3-Oct-2-enyl-oxiranyl)-octanoic acid

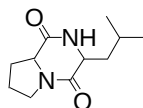
$C_{18}H_{32}O_3$
Exact Mass: 296.24
Mol. Wt.: 296.44
m/e:
C, 72.93; H, 10.88; O, 16.19

27



$C_{20}H_{30}O_{13}$
Exact Mass: 478.17
Mol. Wt.: 478.44
m/e: 478.17 (100.0%), 479.17 (23.2%), 480.17 (2.6%), 480.18 (2.6%)
C, 50.21; H, 6.32; O, 43.47

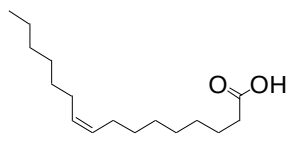
28



3-Isobutyl-hexahydro-pyrrolo[1,2-a]pyrazine-1,4-dione

$C_{11}H_{18}N_2O_2$
Exact Mass: 210.14
Mol. Wt.: 210.27
m/e: 210.14 (100.0%), 211.14 (12.6%), 212.14 (1.2%)
C, 62.83; H, 8.63; N, 13.32; O, 15.22

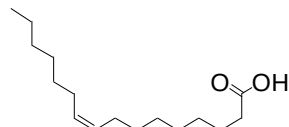
29



Hexadec-9-enoic acid

$C_{16}H_{30}O_2$
Exact Mass: 254.22
Mol. Wt.: 254.41
m/e: 254.22 (100.0%), 255.23 (18.3%), 256.23 (2.0%)
C, 75.54; H, 11.89; O, 12.58

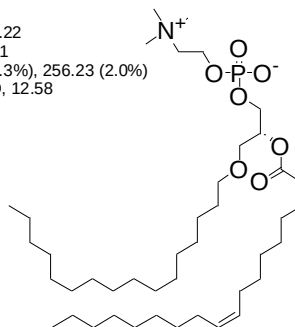
30



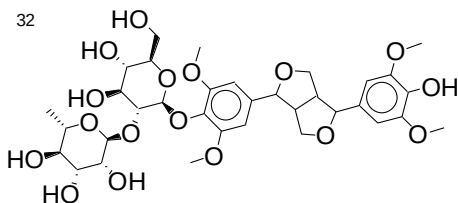
Hexadec-9-enoic acid

$C_{16}H_{30}O_2$
Exact Mass: 254.22
Mol. Wt.: 254.41
m/e: 254.22 (100.0%), 255.23 (18.3%), 256.23 (2.0%)
C, 75.54; H, 11.89; O, 12.58

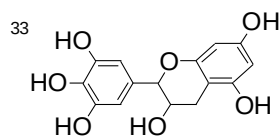
31



$C_{42}H_{84}NO_7P$
Exact Mass: 745.60
Mol. Wt.: 746.09
m/e: 745.60 (100.0%), 746.60 (48.6%), 747.61 (11.4%), 748.61 (2.4%), 747.60 (1.6%)
C, 67.61; H, 11.35; N, 1.88; O, 15.01; P, 4.15

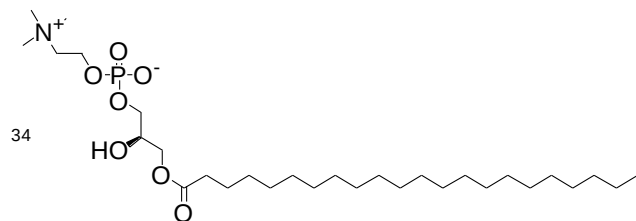


$C_{34}H_{46}O_{17}$
Exact Mass: 726.27
Mol. Wt.: 726.72
m/e: 726.27 (100.0%), 727.28 (39.2%), 728.28 (10.9%), 729.28 (2.2%)
C, 56.19; H, 6.38; O, 37.43

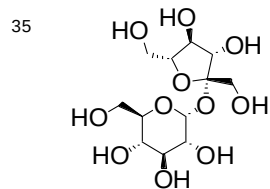


2-(3,4,5-Trihydroxy-phenyl)-chroman-3,5,7-triol

$C_{15}H_{14}O_7$
Exact Mass: 306.07
Mol. Wt.: 306.27
m/e:
C, 58.82; H, 4.61; O, 36.57

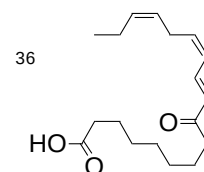


$C_{30}H_{62}NO_7P$
Exact Mass: 579.43
Mol. Wt.: 579.79
m/e: 579.43 (100.0%), 580.43 (34.6%), 581.43 (7.0%)
C, 62.15; H, 10.78; N, 2.42; O, 19.32; P, 5.34
 $C_{109}H_{172}NO_4P$
Exact Mass: 2246.09
Mol. Wt.: 2247.49
m/e:
C, 58.25; H, 7.71; N, 0.62; O, 32.03; P, 1.38



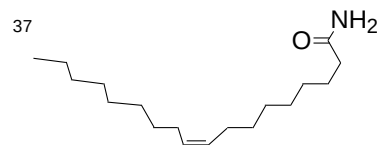
2-(3,4-Dihydroxy-2,5-bis-hydroxymethyl-tetrahydro-furan-2-yloxy)-6-hydroxymethyl-tetrahydro-pyran-3,4,5-triol

$C_{12}H_{22}O_{11}$
Exact Mass: 342.12
Mol. Wt.: 342.30
m/e:
C, 42.11; H, 6.48; O, 51.42



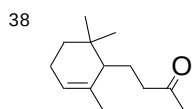
9-Oxo-octadeca-10,12,15-trienoic acid

$C_{18}H_{28}O_3$
Exact Mass: 292.20
Mol. Wt.: 292.41
m/e: 292.20 (100.0%), 293.21 (20.6%), 294.21 (2.6%)
C, 73.93; H, 9.65; O, 16.41



Octadec-9-enoic acid amide

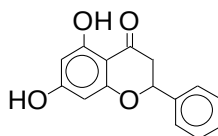
$C_{18}H_{35}NO$
Exact Mass: 281.27
Mol. Wt.: 281.48
m/e: 281.27 (100.0%), 282.28 (20.6%), 283.28 (2.2%)
C, 76.81; H, 12.53; N, 4.98; O, 5.68



4-(2,6,6-Trimethyl-cyclohex-2-enyl)-butan-2-one

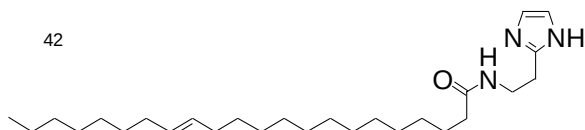
$C_{13}H_{22}O$
Exact Mass: 194.17
Mol. Wt.: 194.31
m/e:
C, 80.35; H, 11.41; O, 8.23

41



$C_{15}H_{12}O_4$
Exact Mass: 256.07
Mol. Wt.: 256.25
m/e: 256.07 (100.0%), 257.08 (17.0%), 258.08 (2.2%)
C, 70.31; H, 4.72; O, 24.97

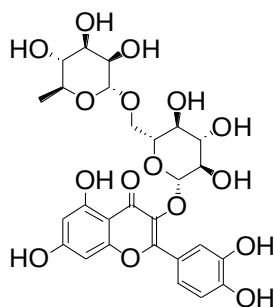
42



Docos-14-enoic acid [2-(1H-imidazol-2-yl)-ethyl]-amide

$C_{27}H_{49}N_3O$
Exact Mass: 431.39
Mol. Wt.: 431.70
m/e: 431.39 (100.0%), 432.39 (30.8%), 433.39 (4.9%), 432.38 (1.1%)
C, 75.12; H, 11.44; N, 9.73; O, 3.71

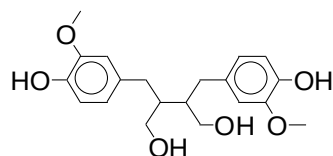
39



2-(3,4-Dihydroxy-phenyl)-5,7-dihydroxy-3-[3,4,5-trihydroxy-6-(3,4,5-trihydroxy-6-methyl-tetrahydro-pyran-2-yloxymethyl)-tetrahydro-pyran-2-yloxy]-chromen-4-one

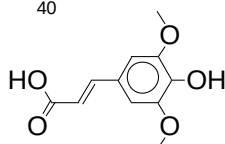
$C_{27}H_{30}O_{16}$
Exact Mass: 610.15
Mol. Wt.: 610.52
m/e:
C, 53.12; H, 4.95; O, 41.93

43



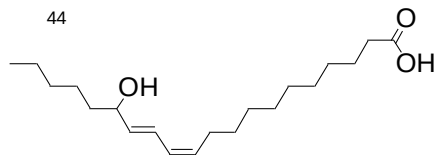
$C_{19}H_{31}O_6$
Exact Mass: 355.21
Mol. Wt.: 355.45
m/e: 355.21 (100.0%), 356.22 (21.8%), 357.22 (3.5%)
C, 64.20; H, 8.79; O, 27.01

40



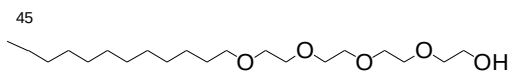
$C_{11}H_{12}O_5$
Exact Mass: 224.07
Mol. Wt.: 224.21
m/e: 224.07 (100.0%), 225.07 (12.6%), 226.07 (1.0%)
C, 58.93; H, 5.39; O, 35.68

44



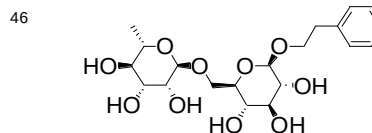
15-Hydroxy-icosa-11,13-dienoic acid

$C_{20}H_{36}O_3$
Exact Mass: 324.27
Mol. Wt.: 324.50
m/e: 324.27 (100.0%), 325.27 (22.9%), 326.27 (3.0%)
C, 74.03; H, 11.18; O, 14.79



2-[2-[2-(2-Dodecyloxy-ethoxy)-ethoxy]-ethoxy]-ethanol

$C_{26}H_{42}O_5$
Exact Mass: 362.30
Mol. Wt.: 362.54
m/e:
C, 66.26; H, 11.68; O, 22.07

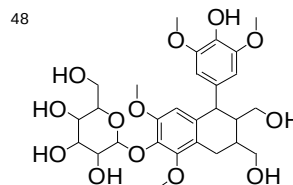


$C_{19}H_{27}O_{10}$
Exact Mass: 415.16
Mol. Wt.: 415.41
m/e: 415.16 (100.0%), 416.16 (21.5%), 417.17 (2.3%), 417.16 (2.0%)
C, 54.93; H, 6.55; O, 38.51



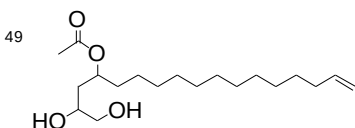
Docos-13-enoic acid amide

$C_{22}H_{43}NO$
Exact Mass: 337.33
Mol. Wt.: 337.58
m/e: 337.33 (100.0%), 338.34 (25.2%), 339.34 (3.2%)
C, 78.27; H, 12.84; N, 4.15; O, 4.74



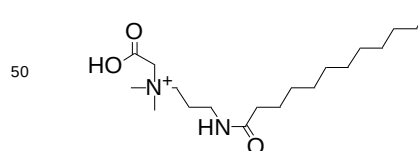
2-[5-(4-Hydroxy-3,5-dimethoxy-phenyl)-6,7-bis-hydroxymethyl-1,3-dimethoxy-5,6,7,8-tetrahydro-naphthalen-2-yloxy]-6-hydroxymethyl-tetrahydro-pyran-3,4,5-triol

$C_{28}H_{38}O_{13}$
Exact Mass: 582.23
Mol. Wt.: 582.59
m/e:
C, 57.72; H, 6.57; O, 35.70



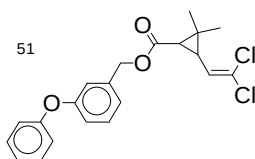
Acetic acid 1-(2,3-dihydroxy-propyl)-tetradec-13-enyl ester

$C_{19}H_{36}O_4$
Exact Mass: 328.26
Mol. Wt.: 328.49
m/e: 328.26 (100.0%), 329.26 (21.1%), 330.27 (3.1%)
C, 69.47; H, 11.05; O, 19.48

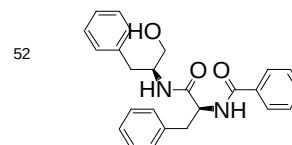


Carboxymethyl-(3-dodecanoylamino-propyl)-dimethyl-ammonium

$C_{19}H_{39}N_2O_3^+$
Exact Mass: 343.30
Mol. Wt.: 343.52
m/e: 343.30 (100.0%), 344.30 (21.8%), 345.30 (2.9%)
C, 66.43; H, 11.44; N, 8.15; O, 13.97

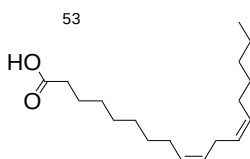


$C_{21}H_{20}Cl_2O_3$
Exact Mass: 390.08
Mol. Wt.: 391.29
m/e: 390.08 (100.0%), 392.08 (64.6%), 391.08 (23.5%), 393.08 (15.2%), 394.07 (10.2%), 392.09 (2.7%), 395.08 (2.5%), 394.08 (2.1%)
C, 64.46; H, 5.15; Cl, 18.12; O, 12.27



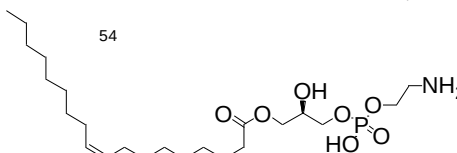
N-[1-(1-Hydroxymethyl-2-phenyl-ethyl-carbamoyl)-2-phenyl-ethyl]-benzamide

$C_{25}H_{26}N_2O_3$
Exact Mass: 402.19
Mol. Wt.: 402.49
m/e:
C, 74.60; H, 6.51; N, 6.96; O, 11.93



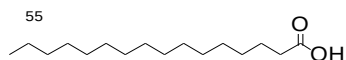
Octadeca-9,12-dienoic acid

$C_{18}H_{32}O_2$
Exact Mass: 280.24
Mol. Wt.: 280.45
m/e: 280.24 (100.0%), 281.24 (20.1%), 282.25 (2.0%)
C, 77.09; H, 11.50; O, 11.41



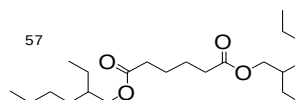
Octadec-9-enoic acid 3-[(2-amino-ethoxy)-hydroxy-phosphoryloxy]-2-hydroxy-propyl ester

$C_{23}H_{46}NO_7P$
Exact Mass: 479.30
Mol. Wt.: 479.59
m/e: 479.30 (100.0%), 480.30 (26.0%), 481.31 (4.8%)
C, 57.60; H, 9.67; N, 2.92; O, 23.35; P, 6.46



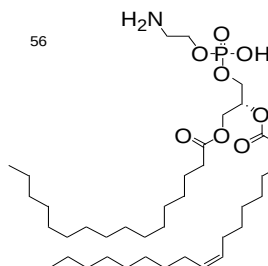
Hexadecanoic acid

$C_{16}H_{32}O_2$
Exact Mass: 256.24
Mol. Wt.: 256.42
m/e: 256.24 (100.0%), 257.24 (17.9%), 258.25 (1.6%)
C, 74.94; H, 12.58; O, 12.48



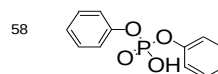
Hexanedioic acid bis-(2-ethyl-hexyl) ester

$C_{22}H_{42}O_4$
Exact Mass: 370.31
Mol. Wt.: 370.57
m/e: 370.31 (100.0%), 371.31 (25.3%), 372.32 (3.1%)
C, 71.31; H, 11.42; O, 17.27



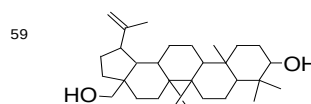
Octadec-9-enoic acid 1-[(2-amino-ethoxy)-hydroxy-phosphoryloxymethyl]-2-hexadecanoyloxy-ethyl ester

$C_{39}H_{74}NO_8P$
Exact Mass: 717.53
Mol. Wt.: 718.00
m/e: 717.53 (100.0%), 718.53 (43.7%), 719.54 (11.4%), 720.54 (2.1%), 718.54 (1.5%)
C, 65.24; H, 10.67; N, 1.95; O, 17.83; P, 4.31



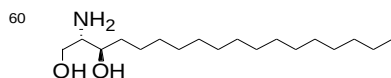
Phosphoric acid diphenyl ester

$C_{12}H_{10}O_4P$
Exact Mass: 250.04
Mol. Wt.: 250.19
m/e: 250.04 (100.0%), 251.04 (13.5%)
C, 57.61; H, 4.43; O, 25.58; P, 12.38



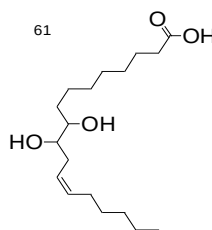
3a-Hydroxymethyl-1-isopropenyl-5a,5b,8,8,11a-pentamethyl-icosahydro-cyclopenta[a]chrysen-9-ol

$C_{30}H_{50}O_2$
Exact Mass: 442.38
Mol. Wt.: 442.72
m/e: 442.38 (100.0%), 443.38 (33.4%), 444.39 (6.1%)
C, 81.39; H, 11.38; O, 7.23



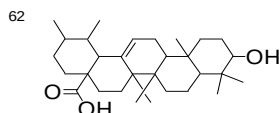
2-Amino-octadecane-1,3-diol

$C_{19}H_{39}NO_2$
Exact Mass: 301.30
Mol. Wt.: 301.51
m/e: 301.30 (100.0%), 302.30 (21.1%), 303.30 (2.4%)
C, 71.70; H, 13.04; N, 4.65; O, 10.61



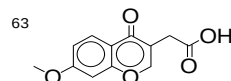
9,10-Dihydroxy-octadec-12-enoic acid

$C_{18}H_{34}O_4$
Exact Mass: 314.25
Mol. Wt.: 314.46
m/e: 314.25 (100.0%), 315.25 (20.7%), 316.25 (2.7%)
C, 68.75; H, 10.90; O, 20.35

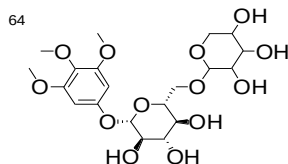


10-Hydroxy-1,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-octadecahydro-2H-picene-4a-carboxylic acid

$C_{30}H_{48}O_3$
Exact Mass: 456.36
Mol. Wt.: 456.70
m/e: 456.36 (100.0%), 457.36 (33.5%), 458.37 (5.7%)
C, 78.90; H, 10.59; O, 10.51

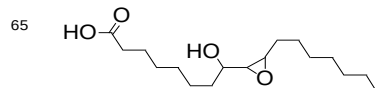


$C_{12}H_{18}O_5$
Exact Mass: 234.05
Mol. Wt.: 234.20
m/e: 234.05 (100.0%), 235.06 (13.7%), 236.06 (1.9%)
C, 61.54; H, 4.30; O, 34.16



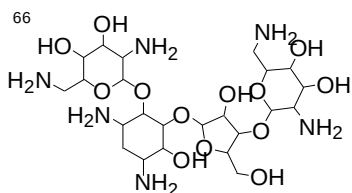
2-(3,4,5-Trihydroxy-tetrahydro-pyran-2-yloxymethyl)-6-(3,4,5-trimethoxy-phenoxy)-tetrahydro-pyran-3,4,5-triol

$C_{20}H_{36}O_{10}$
Exact Mass: 478.17
Mol. Wt.: 478.44
m/e:
C, 50.21; H, 6.32; O, 43.47

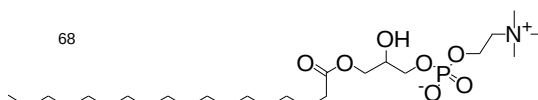


8-Hydroxy-8-(3-octyl-oxiranyl)-octanoic acid

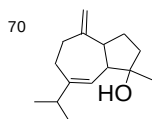
$C_{12}H_{18}O_5$
Exact Mass: 314.25
Mol. Wt.: 314.46
m/e: 314.25 (100.0%), 315.25 (20.7%), 316.25 (2.7%)
C, 68.75; H, 10.90; O, 20.35



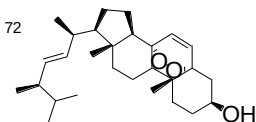
$C_{23}H_{46}N_6O_{13}$
Exact Mass: 614.31
Mol. Wt.: 614.64
m/e: 614.31 (100.0%), 615.32 (26.8%), 616.32 (6.1%), 615.31 (2.2%), 617.32 (1.0%)
C, 44.94; H, 7.54; N, 13.67; O, 33.84



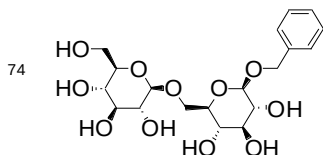
$C_{28}H_{48}NO_7P$
Exact Mass: 517.32
Mol. Wt.: 517.64
m/e: 517.32 (100.0%), 518.32 (29.9%), 519.32 (5.6%)
C, 60.33; H, 9.35; N, 2.71; O, 21.64; P, 5.98



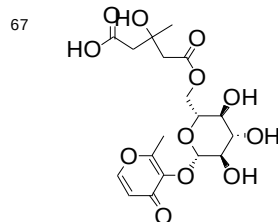
7-Isopropyl-1-methyl-4-methylene-1,2,3,3a,4,5,6,8a-octahydro-azulen-1-ol
 $C_{15}H_{24}O$
Exact Mass: 220.18
Mol. Wt.: 220.35
m/e: 220.18 (100.0%), 221.19 (17.1%), 222.19 (1.6%)
C, 81.76; H, 10.98; O, 7.26



$C_{26}H_{44}O_3$
Exact Mass: 428.33
Mol. Wt.: 428.65
m/e: 428.33 (100.0%), 429.33 (31.3%), 430.34 (4.9%)
C, 78.46; H, 10.35; O, 11.20

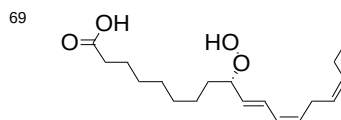


$C_{19}H_{26}O_{11}$
Exact Mass: 432.16
Mol. Wt.: 432.42
m/e: 432.16 (100.0%), 433.17 (22.0%), 434.17 (4.5%)
C, 52.77; H, 6.53; O, 40.70



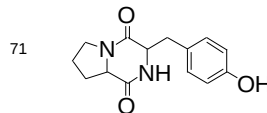
3-Hydroxy-3-methyl-pentanedioic acid mono-[3,4,5-trihydroxy-6-(2-methyl-4-oxo-4H-pyran-3-yloxy)-tetrahydro-pyran-2-ylmethyl] ester

$C_{18}H_{24}O_{12}$
Exact Mass: 432.13
Mol. Wt.: 432.38
m/e: 432.13 (100.0%), 433.13 (20.9%), 434.13 (4.4%)
C, 50.00; H, 5.59; O, 44.40



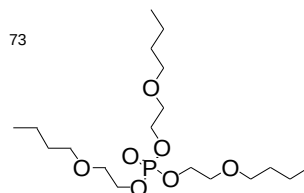
9-Hydroperoxy-octadeca-10,12,15-trienoic acid

$C_{18}H_{30}O_3$
Exact Mass: 310.21
Mol. Wt.: 310.43
m/e: 310.21 (100.0%), 311.22 (20.6%), 312.22 (2.8%)
C, 69.64; H, 9.74; O, 20.62



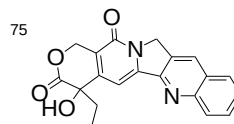
3-(4-Hydroxy-benzyl)-hexahydro-pyrrolo[1,2-a]pyrazine-1,4-dione

$C_{14}H_{16}N_2O_3$
Exact Mass: 260.12
Mol. Wt.: 260.29
m/e:
C, 64.60; H, 6.20; N, 10.76; O, 18.44



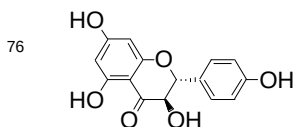
Phosphoric acid tris-(2-butoxy-ethyl) ester

$C_{28}H_{38}O_7P$
Exact Mass: 398.24
Mol. Wt.: 398.47
m/e: 398.24 (100.0%), 399.25 (20.9%), 400.25 (3.5%)
C, 54.26; H, 9.87; O, 28.11; P, 7.77



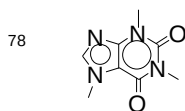
4-Ethyl-4-hydroxy-1,12-dihydro-4H-2-oxa-6,12a-diaza-dibenzo[*b,h*]fluorene-3,13-dione
#8: Please note: Replacement nomenclature used: fusion ring name maybe better;
Note for CAS rings: this class is not yet supported, Beilstein ring name(s) generated

$C_{20}H_{10}N_2O_3$
Exact Mass: 348.11
Mol. Wt.: 348.35
m/e:
C, 68.96; H, 4.63; N, 8.04; O, 18.37

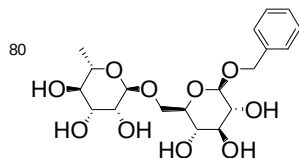


3,5,7-Trihydroxy-2-(4-hydroxy-phenyl)-chroman-4-one

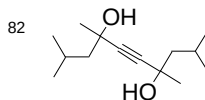
$C_{15}H_{10}O_6$
Exact Mass: 288.06
Mol. Wt.: 288.25
m/e: 288.06 (100.0%), 289.07 (17.1%), 290.07 (2.6%)
C, 62.50; H, 4.20; O, 33.30



$C_8H_{10}N_4O_2$
Exact Mass: 194.08
Mol. Wt.: 194.19
m/e: 194.08 (100.0%), 195.08 (10.5%)
C, 49.48; H, 5.19; N, 28.85; O, 16.48

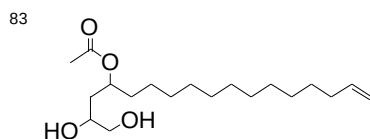


$C_{19}H_{28}O_{10}$
Exact Mass: 416.17
Mol. Wt.: 416.42
m/e: 416.17 (100.0%), 417.17 (22.0%), 418.17 (4.1%)
C, 54.80; H, 6.78; O, 38.42



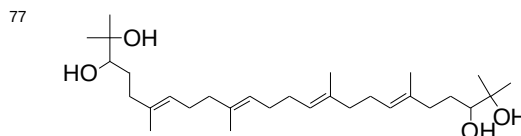
2,4,7,9-Tetramethyl-dec-5-yne-4,7-diol
#3: Please note: Alphabetic order of prefixes ignored while selecting parent chain

$C_{14}H_{26}O_2$
Exact Mass: 226.19
Mol. Wt.: 226.36
m/e: 226.19 (100.0%), 227.20 (16.0%), 228.20 (1.6%)
C, 74.29; H, 11.58; O, 14.14



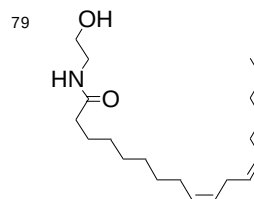
Acetic acid 1-(2,3-dihydroxy-propyl)-tetradec-13-enyl ester

$C_{19}H_{38}O_4$
Exact Mass: 328.26
Mol. Wt.: 328.49
m/e: 328.26 (100.0%), 329.26 (21.1%), 330.27 (3.1%)
C, 69.47; H, 11.05; O, 19.48



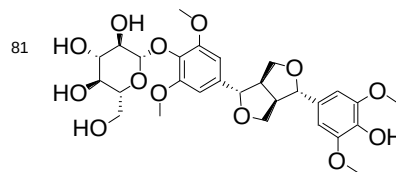
2,6,10,15,19,23-Hexamethyl-tetracos-6,10,14,18-tetraene-2,3,22,23-tetraol
#3: Please note: Alphabetic order of prefixes ignored while selecting parent chain

$C_{30}H_{54}O_4$
Exact Mass: 478.40
Mol. Wt.: 478.75
m/e: 478.40 (100.0%), 479.41 (34.3%), 480.41 (6.5%)
C, 75.26; H, 11.37; O, 13.37



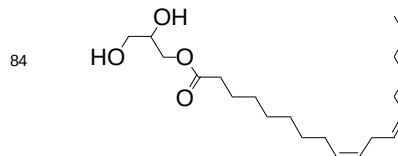
Octadeca-9,12-dienoic acid (2-hydroxy-ethyl)-amide

$C_{20}H_{37}NO_2$
Exact Mass: 323.28
Mol. Wt.: 323.51
m/e: 323.28 (100.0%), 324.29 (22.9%), 325.29 (2.9%)
C, 74.25; H, 11.53; N, 4.33; O, 9.89



2-{4-[4-(4-Hydroxy-3,5-dimethoxy-phenyl)-tetrahydro-furo[3,4-c]furan-1-yl]-2,6-dimethoxy-phenoxy}-6-hydroxymethyl-tetrahydro-pyran-3,4,5-triol

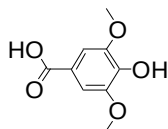
$C_{28}H_{38}O_{13}$
Exact Mass: 580.22
Mol. Wt.: 580.58
m/e: 580.22
C, 57.93; H, 6.25; O, 35.83



Octadeca-9,12-dienoic acid 2,3-dihydroxy-propyl ester

$C_{21}H_{38}O_4$
Exact Mass: 354.28
Mol. Wt.: 354.52
m/e: 354.28 (100.0%), 355.28 (24.1%), 356.28 (3.4%)
C, 71.14; H, 10.80; O, 18.05

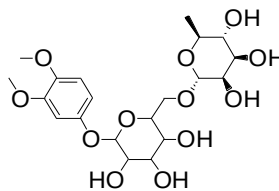
85



4-Hydroxy-3,5-dimethoxy-benzoic acid

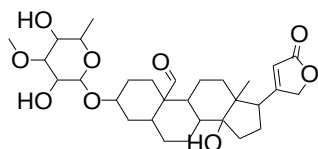
$C_9H_{10}O_5$
 Exact Mass: 198.05
 Mol. Wt.: 198.17
 m/e: 198.05 (100.0%), 199.06 (10.4%), 200.06 (1.5%)
 C, 54.55; H, 5.09; O, 40.37

86



$C_{20}H_{30}O_{12}$
 Exact Mass: 462.17
 Mol. Wt.: 462.44
 m/e: 462.17 (100.0%), 463.18 (23.2%), 464.18 (5.0%)
 C, 51.94; H, 6.54; O, 41.52

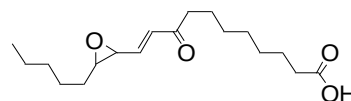
87



3-(3,5-Dihydroxy-4-methoxy-6-methyl-tetrahydro-pyran-2-yloxy)-14-hydroxy-13-methyl-17-(5-oxo-2,5-dihydro-furan-3-yl)-hexadecahydro-cyclopenta[a]phenanthrene-10-carbaldehyde

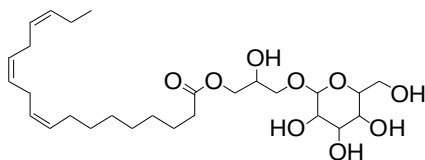
$C_{30}H_{44}O_9$
 Exact Mass: 548.30
 Mol. Wt.: 548.66
 m/e:
 C, 65.67; H, 8.08; O, 26.24

88



9-Oxo-11-(3-pentyl-oxiranyl)-undec-10-enoic acid

$C_{19}H_{30}O_4$
 Exact Mass: 310.21
 Mol. Wt.: 310.43
 m/e: 310.21 (100.0%), 311.22 (20.6%), 312.22 (2.8%)
 C, 69.64; H, 9.74; O, 20.62



Octadeca-9,12,15-trienoic acid 2-hydroxy-3-(3,4,5-trihydroxy-6-hydroxymethyl-tetrahydro-pyran-2-yloxy)-propyl ester

$C_{27}H_{46}O_9$
 Exact Mass: 514.31
 Mol. Wt.: 514.65
 m/e: 514.31 (100.0%), 515.32 (31.1%), 516.32 (6.5%)
 C, 63.01; H, 9.01; O, 27.98

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