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Phytochemical Screening and Gc-Ms Profile of *Melastomastrum Capitatum* A. & R. Fern. Methanol Root Extract for Bioactive Anti-Brain Tumor Compounds

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Abstract

Melastomastrum capitatum is a tropical fruit tree of considerable economic importance, originating from West and tropical Africa. Belonging to the Melastomataceae family, M. capitatum has been traditionally used to address ailments such as cancer, stomachache, diabetes, pain, and inflammation. The current study aimed to analyze the phytochemical constituents of the methanol extract from the root of M. capitatum using phytochemical assessment and gas chromatography-mass spectrometry (GC–MS). The phytochemical analysis revealed seven compounds, including alkaloids, saponins, flavonoids, steroids, cardiac glycosides, and terpenoids, with saponins being the most abundant at 51.8%. The GC–MS analysis detected many bioactive compounds that such as phthalic acid derived compounds and others which may contribute to various pharmacological effects. Linoleic acid was the most prevalent compound found, known for its antioxidant, anti-inflammatory, and antidiabetic properties. Phthalic acid derivatives were also noted for their antimicrobial, anticancer, antioxidant, and anti-inflammatory effects. Additionally, other noteworthy compounds such as 3,4-Dihydroxyphenylglycol (4TMS derivative) and 2,4-Pentadien-1-ol, 3-propyl- were identified, recognized for their antioxidant and anticancer capabilities, respectively. These results lend support to the traditional use of M. capitatum for treating various health issues.

Keywords: *Melastomastrum capitatum, phytochemical screening, GC-MS analysis, bioactive compounds, anti-brain tumor potential.*

1. Introduction

Medicinal plants are a valuable source for both traditional and modern medicine, with approximately 80% of the rural population relying on them for primary healthcare [1]. Despite significant advancements in synthetic organic medicinal products in the twentieth century, more than a quarter of the medications prescribed in developed nations still originate from plants. These plants have been recognized for thousands of years and are highly regarded worldwide as abundant sources of therapeutic agents for disease prevention and treatment. According to the World Health Organization (WHO), around four billion people, 80% of the global population, utilize herbal medicines as part of their primary healthcare [2]. Various compounds can be extracted and analyzed from plants for research and the development of new pharmaceutical treatments. However, a major challenge for researchers is that a single plant may contain numerous bioactive compounds. Identifying these compounds and understanding their biological activities is essential for clarifying issues related to toxicity, side effects, proper dosages, and effective extraction techniques [3].

Melastomastrum capitatum is a shrub that can reach heights of up to 1.25 meters, typically found in dry areas and along stream banks in Nigeria, particularly on the Mambila Plateau in Taraba State [4]. The Fulani tribe in this region refers to it as "*Belkon*" and utilizes its leaves in traditional medicine for treating cancer and various other ailments. The plant has a flavor that ranges from sweet to sour. In Ivory Coast, a diluted leaf sap is used as a sedative. Additionally, its leaves are known in traditional medicine to lower cholesterol, provide pain relief, and cleanse blood vessels. In the southern

regions of Nigeria, it is commonly employed for wound healing. The leaves have a distinctive appearance, growing in opposite pairs and typically exhibiting sweet and sour tastes. Research on *M. capitatum* is still in the early stages, and no specific compounds have yet been isolated from any part of the plant. However, preliminary phytochemical analysis of the leaf methanol extract has indicated the presence of glycosides, alkaloids, and carbohydrates[5].

The plant typically thrives year-round along the edges of water channels and valleys in the Mambila Plateau, specifically in the Sarduana Local Government Area of Taraba, where it is among the most prevalent shrubs, often featuring vibrantly colored leaves[5]. The availability of water and the cool climate in this region significantly contribute to its growth. Besides the Mambila Plateau, the plant also flourishes in Ogurugu Uzo-Uwani Local Government Area of Enugu State, where it is mainly found in marshlands and damp areas, particularly near shallow streams. Additionally, it can be spotted in Ibaji Local Government Area of Kogi State, Borgu Local Government Area of Niger State, the southern region of Kaduna State, parts of Northern and Southern Borno, Edo State, and in the southwestern Nigerian states of Ondo, Ekiti, Lagos, Oyo, and Osun[6].

The leaves are primarily utilized in traditional medicine for purposes such as blood purification, treating stomach pain, and serving as an antitumor and anticancer agent according to the Fulani tribe, although these claims have yet to be scientifically validated. Research indicates that the leaves possess analgesic, anticancer, antioxidant and anti-inflammatory properties, as well as anti-hypercholesterolemic effects in mice[7]. However, other potential uses of the plant remain undocumented due to limited research, as it is still relatively unexplored in the fields of plant science and pharmacognosy. Consequently, this study was conducted to identify the key bioactive compounds present in the methanol extract of *M. capitatum* root using gas chromatography/mass spectrometry (GC-MS). This marks the first effort to isolate compounds from *M. capitatum* root.

2. Materials And Methods

2.1. Materials

The following chemicals and equipment were utilized in this research: solvents of varying polarities (n-hexane, ethyl acetate, n-butanol, and methanol; Sigma Aldrich St Lous Mo, USA), GEMINI-20 portal milligram scale (AWS, China), separating funnels with a capacity of 1000 mL, a rotary evaporator, TLC plates made of silica gel 60 F254 measuring 20 × 20 cm (Merck, Germany), a glass column measuring 35 × 950 mm, and a GC–MS system (7890 GC system; Agilent Technologies), among other reagents and apparatus.

2.2. Methods

2.2.1 Collection and identification of plant material

Fresh roots of Melastomastrum capitatum were gathered in the evening from the banks of the Fori River in Maiduguri, Nigeria, in February 2025, to align with the timing used by traditional medicine practitioners when harvesting the plant for therapeutic purposes. The plant was verified and assigned a voucher specimen number "UMM/FPH/MEA/001" at the herbarium of the Department of Pharmacognosy, Faculty of Pharmacy, University of Maiduguri, by taxonomist Dr. C.A. Ukwubile.

2.2.2. Preparation of plant material

The freshly collected roots of *M. capitatum* were dried in the shade for two weeks. They were then ground into a fine powder using an electronic blender (Model 5000 MH, Japan). The powdered material was passed through a sieve with a 20-mesh size to achieve a finer consistency and eliminate any undesirable particles. The weight of the powder was recorded using a scale balance to determine the initial mass. Finally, the powdered plant material was stored in a clean, dry bag for future use[8].

2.2.3. Extraction of plant material

A total of 800 g of powdered *M. capitatum* roots was subjected to defatting with petroleum ether (80 °C) to eliminate fat and latex. The remaining defatted plant material was then subjected to extraction using a Soxhlet apparatus with methanol at 40 °C for 12 hours to obtain the methanol extract. Methanol was chosen for its capability to extract both polar and non-polar components from the roots. The solvent was replaced regularly until there was no further coloration observed. The resulting extract was filtered using Whatman filter paper No. 1. Subsequently, the filtrate was concentrated under reduced pressure using a rotary evaporator (model 503, Auxilab, France). The final weight of the extract was recorded, and the percentage yield was calculated based on the initial weight of the powdered leaves as follows:

$$\text{Yield (\%)} = \frac{Final\ weight\ of\ extract}{Initial\ weight\ of\ powdered\ roots} x\ 100$$

The dried extract was then stored in a clean sample bottle and kept in a refrigerator at 4 °C until use.

2.2.4. Liquid-liquid fractionation of M. capitatum root extract

The methanol extract of *M. capitatum* roots was subjected to liquid-liquid fractionation using solvents arranged in increasing order of polarity: n-hexane, ethyl acetate, n-butanol, and methanol. A total of 200 grams of root extract was mixed with 300 mL of methanol and 700 mL of distilled water in a 1000 mL separating funnel. The mixture was shaken vigorously until the extract was fully dissolved. It was then partitioned three times with 300 mL of each solvent, resulting in the collection of the filtrates. These filtrates were concentrated under reduced pressure using a rotary evaporator, yielding a dark, jelly-like extract. The final extracts were weighed, labeled, and stored in clean sample bottles [8].

2.2.5. Phytochemical screening

The phytochemical screening of *M. capitatum* root extract fractions of n-hexane (HF), ethyl acetate (EF), n-butanol (BF), and methanol (MF), was conducted to identify the presence of various bioactive compounds. Standard qualitative phytochemical tests were performed following established protocols to detect the presence of alkaloids, flavonoids, tannins, saponins, terpenoids, glycosides, phenols, and steroids [9].

2.2.5.1. Alkaloids test

Wagner's test: Few drops of Wagner's reagent (iodine in potassium iodide) are added to 0.5 g extract. A reddish-brown precipitate indicates the presence of alkaloids.

Dragendorff's test: Few drops of Dragendorff's reagent (bismuth nitrate and potassium iodide) are added to 0.5 g extract. An orange or reddish-brown precipitate confirms the presence of alkaloids.

2.2.5.2. Flavonoids test

Shinoda test: 0.5 g extract is mixed with 5 g of magnesium turnings, followed by the addition of 2 mL of concentrated hydrochloric acid (HCl). The formation of a pink color indicates the presence of flavonoids.

Alkaline reagent test: A few drops of sodium hydroxide (NaOH) solution are added to 0.5 g extract. A yellow coloration that turns colorless upon the addition of 1 mL of dilute acid confirms the presence of flavonoids.

2.2.5.3. Tannins test

Ferric chloride test: A few drops of ferric chloride ($FeCl_3$) solution are added to 0.5 g extract. A blue-black or greenish coloration indicates the presence of tannins.

Lead acetate test: A few drops of lead acetate solution are added to 0.5 g extract. A yellowish or brownish precipitate confirms the presence of tannins.

2.2.5.4. Saponins test

Frothing test: 0.5 g extract is mixed with 5 mL of distilled water and vigorously shaken for 5 min. Persistent froth formation that lasts for a few minutes indicates the presence of saponins.

2.2.5.5. Terpenoids test

Salkowski test: Exactly 0.5 g extract is mixed with 2 mL of chloroform, and 1 mL of concentrated sulfuric acid (H_2SO_4) is carefully added to form a layer. A reddish-brown coloration at the interface indicates the presence of terpenoids.

Liebermann-Burchard test: 0.5 g extract is dissolved in acetic anhydride and cooled, followed by the addition of one drop of concentrated sulfuric acid. A blue, green, or red coloration confirms the presence of terpenoids.

2.2.5.6. Steroids test

Liebermann-Burchard test: A few drops of acetic anhydride and concentrated sulfuric acid are added to 0.5 g extract. The development of blue or green coloration indicates the presence of steroids.

2.2.5.7. Glycosides test

Keller-Killiani test (cardiac glycosides): 0.5 g extract is mixed with glacial acetic acid containing ferric chloride, followed by the addition of few drops concentrated sulfuric acid. The appearance of a reddish-brown ring at the interface confirms the presence of glycosides.

Borntrager's test (anthraquinone glycosides): 0.5 g extract is boiled with dilute sulfuric acid, followed by the addition of 5 mL chloroform and 1 mL ammonia. A pink to red coloration in the ammonia layer indicates the presence of anthraquinone glycosides.

2.2.5.8. Phenols test

Ferric chloride test: A few drops of ferric chloride ($FeCl_3$) solution are added to 0.5 g extract. A deep blue or greenish-black coloration indicates the presence of phenolic compounds.

2.2.6. Purification of extract using silica gel column chromatography

A total of 10 grams of the methanol extract was processed using a silica gel column measuring 35 × 950 mm. The elution was performed using a gradient of ethyl acetate and methanol in the following ratios: 95:5, 90:10, 80:20, 70:30, 50:50, and 0:100. In total, 50 fractions were collected and categorized into six groups (I–VI) based on their thin-layer chromatography (TLC) profiles. Each group underwent further purification on a shorter column, resulting in final purified portions labeled as ME I, ME II, ME III, ME IV, ME V, and ME VI. Each isolate was concentrated to dryness, weighed, and stored in ALS vials for future use[10].

2.2.7. GC–MS analysis of methanol fractions of root

The ME I-ME VI (0.1 µL), was dissolved in 5 mL of methanol and injected in an Agilent 7890A GC system coupled with an MS (Agilent technologies, USA) by author injection at the Central Research Laboratory, University of Lagos, Akoka, Lagos Nigeria. The operating conditions of the GC–MS set for the analysis were as follows: oven temperature 50°C for 2 min then 100°C at 10°C/ min and finally increased to 200°C and held isothermally for 10 min. The sample injection was 2 µL and the carrier gas was helium at 1 mL/min. The ionization of the sample components was carried out 70 eV. The total running time of the GC was 24.50 min. NIST14.L library (2018) was then searched to compare the structures of the compounds with that of the NIST database. Compounds were then identified based on the retention times and mass spectra with already known compounds in the NIST library (C:\Database\NIST14.L) [10].

3. Results And Discussion

3.1. Phytochemical and G-MS Analysis of Various Fractions of *M. Capitatum* Root Extract

The methanol fraction (MF) contained the highest concentration of phytochemicals, including alkaloids, flavonoids, tannins, saponins, terpenoids, steroids, glycosides, anthraquinones, coumarins, and carbohydrates, indicating its broad spectrum of bioactive compounds. The n-butanol fraction (BF) also exhibited strong presence of flavonoids, tannins, saponins, phenols, glycosides, and resins, suggesting its suitability for extracting both polar and semi-polar phytochemicals. The ethyl acetate fraction (EF) showed moderate levels of alkaloids, flavonoids, tannins, terpenoids, glycosides, and anthraquinones, indicating its effectiveness in extracting semi-polar compounds. The n-hexane fraction (HF) contained minimal phytochemicals, primarily terpenoids and steroids, which are non-polar compounds commonly soluble in hexane (Table 1).

Table 1. *Phytochemical content of M. capitatum root extracts*

Phytochemical	Tests	HF	EF	BF	MF
Alkaloids	Wagner's, Dragendorff's	-	+	+	++
Flavonoids	Shinoda, Alkaline Reagent	-	+	++	++
Tannins	Ferric Chloride, Lead Acetate	-	+	++	++
Saponins	Frothing	-	+	++	++
Terpenoids	Salkowski, Liebermann-Burchard	+	++	++	++
Steroids	Liebermann-Burchard	+	++	++	++
Phenols	Ferric Chloride	-	+	++	++
Cardiac glycosides	Keller-Killiani	-	+	+	++
Anthraquinones	Borntrager's	-	+	+	++
Coumarins	NaOH	-	+	+	++
Resins	Acetone-HCl	-	-	+	+
Carbohydrates	Molisch's, Fehling's	-	+	++	++
Reducing sugars	Fehling's, Benedict's	-	+	+	++

*Key: **(++)** = strongly present, **(+)** = moderately present, **(-)** = absent. MF: methanol fraction, BF: n-butanol fraction, EF: ethyl acetate fraction, and HF: n-hexane fraction.*

The phytochemical screening of *Melastomastrum capitatum* root extract fractions revealed a diverse range of bioactive compounds with potential therapeutic relevance, particularly in the management of brain tumors and other cancers. The methanol fraction (MF) contained

the highest concentration of phytochemicals, including alkaloids, flavonoids, tannins, saponins, terpenoids, steroids, anthraquinones, coumarins, and carbohydrates, suggesting a broad pharmacological potential. These secondary metabolites have been extensively studied for their anticancer and neuroprotective properties, particularly in targeting signaling pathways involved in tumor progression and resistance.

Alkaloids present in the methanol fraction have demonstrated significant anticancer potential. For instance, vinblastine and vincristine, alkaloids derived from *Catharanthus roseus*, are widely used in chemotherapy due to their ability to disrupt microtubule formation, leading to apoptosis in cancer cells [11]. Similarly, studies have shown that certain alkaloids, such as sanguinarine and berberine, exert cytotoxic effects on glioblastoma multiforme (GBM) by inhibiting key oncogenic pathways, including PI3K/Akt/mTOR and NF-κB signaling [12].

Flavonoids, which were strongly present in the methanol and n-butanol fractions, have been reported to possess potent antioxidant, anti-inflammatory, and anticancer activities. Quercetin and luteolin, for instance, have been shown to induce apoptosis and inhibit the proliferation of glioblastoma cells through modulation of Wnt/β-catenin and MAPK/ERK pathways [13]. Moreover, flavonoids can enhance the efficacy of conventional chemotherapy by reducing drug resistance mechanisms in gliomas [14]. Tannins, detected in significant amounts in the methanol and n-butanol fractions, are polyphenolic compounds known for their anticancer properties. Gallotannins and ellagitannins have been reported to exert cytotoxic effects against brain tumor cells by modulating oxidative stress and inducing mitochondrial dysfunction [15]. Their strong antioxidant activity helps in reducing DNA damage, a key factor in the initiation and progression of brain tumors.

Saponins, which were highly present in methanol and n-butanol fractions, have shown promise in brain tumor research due to their ability to disrupt tumor cell membranes, induce apoptosis, and inhibit angiogenesis. Diosgenin, a well-studied saponin, has been reported to downregulate the expression of vascular endothelial growth factor (VEGF) and matrix metalloproteinases (MMPs), thereby reducing glioma cell invasiveness [16]. Terpenoids and steroids, abundant in the methanol and ethyl acetate fractions, are bioactive compounds known to exhibit anticancer effects through multiple mechanisms. Betulinic acid, a pentacyclic triterpenoid, has been shown to induce apoptosis in glioblastoma cells by activating caspase-dependent pathways and inhibiting HIF-1α-mediated hypoxia adaptation [17]. Steroidal compounds such as withaferin A have also demonstrated significant anticancer potential by inhibiting NF-κB and STAT3 signaling pathways in brain tumor models [18].

Anthraquinones, detected in methanol and ethyl acetate fractions, are known to possess potent cytotoxic and anti-proliferative properties. Emodin, a natural anthraquinone, has been reported to suppress glioblastoma progression by inhibiting Akt and ERK signaling while promoting autophagy-mediated cell death [19]. These findings align with the presence of anthraquinones in *M. capitatum*, suggesting a potential role in brain tumor inhibition. Glycosides, including cardiac glycosides, were present in the methanol and n-butanol fractions, which is significant because these compounds have been explored for their anticancer potential. Cardiac glycosides such as digoxin and ouabain have been shown to induce apoptosis in glioblastoma cells by inhibiting Na+/K+-ATPase and disrupting intracellular ion homeostasis [19].

The n-hexane fraction (HF), which mainly contained terpenoids and steroids, exhibited minimal phytochemical content, suggesting its limited anticancer potential. However, non-polar compounds such as limonene and β-caryophyllene have been reported to possess neuroprotective and anticancer activities through the modulation of oxidative stress and neuroinflammation [20]. Overall, the phytochemical composition of *M. capitatum* root extract fractions suggests a promising role in brain tumor therapy. The methanol and n-butanol fractions, which exhibited the highest concentrations of bioactive compounds, may serve as potential sources for the development of novel anti-glioma and neuroprotective agents. Further studies involving in vitro and *in vivo* models are necessary to validate their therapeutic efficacy and mechanisms of action in brain tumor management.

Similarly, the GC-MS analysis shows interesting bioactive compounds belonging to various classes of compounds (Table 2). For instance, fatty acids (palmitic acid, linoleic acid, oleic

acid) are compounds have been reported to exhibit anti-inflammatory and anticancer properties, particularly in modulating lipid metabolism in cancer cells [21]. Linoleic acid has been shown to inhibit tumor cell proliferation and induce apoptosis in glioblastoma models [22].

Steroids (stigmasterol, β-sitosterol, campesterol) as phytosterols have antitumor effects, modulating cell membrane integrity and apoptosis pathways in brain tumor models [23]. Furthermore, terpenoids (squalene, lupeol, ursolic acid, friedelin) like ursolic acid and lupeol have demonstrated anticancer and anti-inflammatory effects, suppressing NF-κB, Akt, and MAPK pathways in glioblastoma and breast cancer [19]. Flavonoids (5-Hydroxy-7-methoxyflavone) are compounds which have potent antioxidant and anticancer properties, capable of modulating oxidative stress and inflammatory cytokines in brain tumors [24]. It has been reported that vitamin E (α-tocopherol) are known for its neuroprotective and anticancer effects, vitamin E prevents oxidative stress-induced damage in neural cells and glioblastoma cells [25].

Table 2. *GC-MS composition of* M. capitatum *root methanol extract*

Peak no.	Compound name	RT (min)	Peak area (%)	m/z (mol/g)	Molecular formula	Type of compound
1	Hexadecanoic acid	18.52	8.12	256.42	$C_{16}H_{32}O_2$	Fatty acid
2	9,12-Octadecadienoic acid	19.85	12.46	280.45	$C_{18}H_{32}O_2$	Polyunsaturated fatty acid
3	Oleic acid	20.12	10.35	282.47	$C_{18}H_{34}O_2$	Monounsaturated fatty acid
4	Phthalic acid	21.35	7.89	296.53	$C_{20}H_{40}O$	Diterpene alcohol
5	Stigmasterol	22.78	6.54	412.69	$C_{29}H_{48}O$	Steroid
6	β-Sitosterol	23.10	9.76	414.71	$C_{29}H_{50}O$	Phytosterol
7	Squalene	23.95	5.62	410.71	$C_{30}H_{50}$	Triterpene
8	1,2 Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	24.63	4.78	390.56	$C_{24}H_{38}O_4$	Phthalate ester
9	2,3-Dihydroxypropyl elaidate	25.87	3.67	358.56	$C_{21}H_{40}O_4$	Glycolipid
10	Campesterol	26.10	5.25	400.69	$C_{28}H_{48}O$	Phytosterol
11	Lupeol	27.45	6.92	426.72	$C_{30}H_{50}O$	Triterpenoid
12	Urs-12-en-28-oic acid	28.75	7.13	456.70	$C_{30}H_{48}O_3$	Triterpenoid
13	Friedelin	29.38	4.21	426.73	$C_{30}H_{50}O$	Triterpenoid
14	Vitamin E	30.52	3.98	430.72	$C_{29}H_{50}O_2$	Antioxidant
15	5-Hydroxy-7-methoxyflavone	31.89	4.57	300.26	$C_{16}H_{12}O_4$	Flavonoid

RT: retention time and m/z: mass-to-charge ratio.

3.2. Novel Phthalic Acid-Derived Compounds From *M. Capitatum* Ethyl Acetate Fraction with Potential Anti-Tumor Activity

Phthalates (Fig. 1a-i), esters of phthalic acid, have traditionally been studied for their role as plasticizers and their potential endocrine-disruption properties. However, recent research has begun to explore their therapeutic potential, particularly in oncology. Certain phthalate esters have demonstrated cytotoxic activities against cancer cell lines, including those of brain origin. Among these, long-chain and branched phthalates appear to exhibit promising anticancer effects, likely due to their physicochemical properties that enable them to interact with cellular membranes, disrupt signaling pathways, and induce apoptosis[26].

Phthalic acid, 2-ethylhexyl tetradecyl ester ($C_{30}H_{50}O_4$) is a compound characterized by its long, branched alkyl chains, contributing to its high lipophilicity. This property is essential for compounds intended to cross the blood-brain barrier and interact with brain tumor cells. Although specific studies on this exact ester are limited, structurally related compounds such as di-(2-ethylhexyl) phthalate (DEHP) have shown cytotoxic activity against glioblastoma multiforme (GBM) cells. Alkaram et al. [27] demonstrated that DEHP inhibited GBM cell proliferation and induced apoptosis by suppressing the ERK and PI3K/Akt signaling pathways, both of which are crucial for brain tumor cell survival and proliferation. This suggests that derivatives like 2-ethylhexyl tetradecyl ester may exert similar effects through mitochondrial damage, reactive oxygen species (ROS) generation, and disruption of lipid-based signaling domains.

Phthalic acid, butyl undecyl ester is another long-chain phthalate with a balance of hydrophobic and hydrophilic characteristics, making it a candidate for cellular uptake and interaction with

brain tumor cells. The undecyl chain enhances its membrane affinity, potentially enabling the compound to disrupt mitochondrial function and interfere with cellular metabolism. Mohammad et al. [28] reported that certain phthalate derivatives could exhibit moderate anticancer effects through oxidative stress induction and inhibition of metabolic enzymes in cancer cells. Although specific data on butyl undecyl ester and brain tumors are lacking, its structural properties and lipophilic profile suggest it may act similarly to known cytotoxic phthalates.

Similarly, phthalic acid, butyl tetradecyl ester contains a tetradecyl chain, which further increases its membrane-permeating capacity. Long-chain esters like this may interact with the lipid rafts of glioma or neuroblastoma cells, affecting membrane integrity and inducing apoptosis. Rahman et al. [26] highlighted the potential of phthalate esters to modulate caspase activity, interfere with cell cycle progression, and cause mitochondrial depolarization. These mechanisms are particularly relevant in brain tumors, where apoptosis evasion and mitochondrial dysregulation are hallmarks of disease progression.

Lastly, phthalic acid, dodecyl octyl ester is a compound with two long hydrophobic chains, suggesting a high affinity for cellular lipid environments. Its structural similarity to other cytotoxic phthalates positions it as a potential candidate for targeting lipid-rich microdomains in glioma and neuroblastoma cells. Liu et al. [29] demonstrated that long-chain phthalates exert selective toxicity in neuroblastoma and glioma cells by inducing DNA fragmentation, ROS production, and cell cycle arrest. These activities, coupled with their ability to penetrate the blood-brain barrier, make such compounds attractive as potential lead structures for anti-brain tumor therapeutics.

In conclusion, while phthalates have historically been viewed through the lens of toxicity, certain derivatives—especially those with long and branched alkyl chains—may offer novel opportunities for brain tumor treatment. Their lipophilic nature facilitates cell entry and mitochondrial interaction, leading to oxidative stress, apoptosis, and inhibition of pro-survival pathways. Although more in-depth studies, including in vivo evaluations and toxicity profiling, are necessary, the aforementioned phthalates present a promising frontier in brain tumor pharmacology.

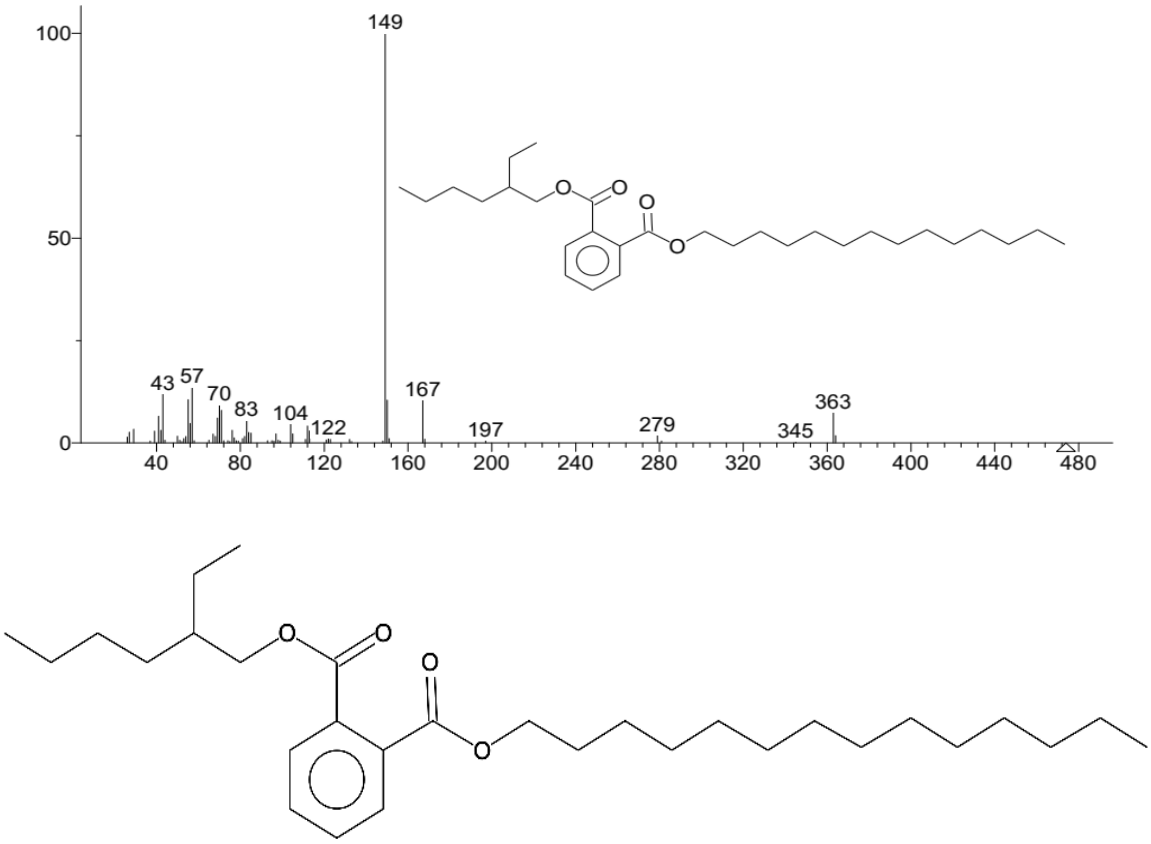
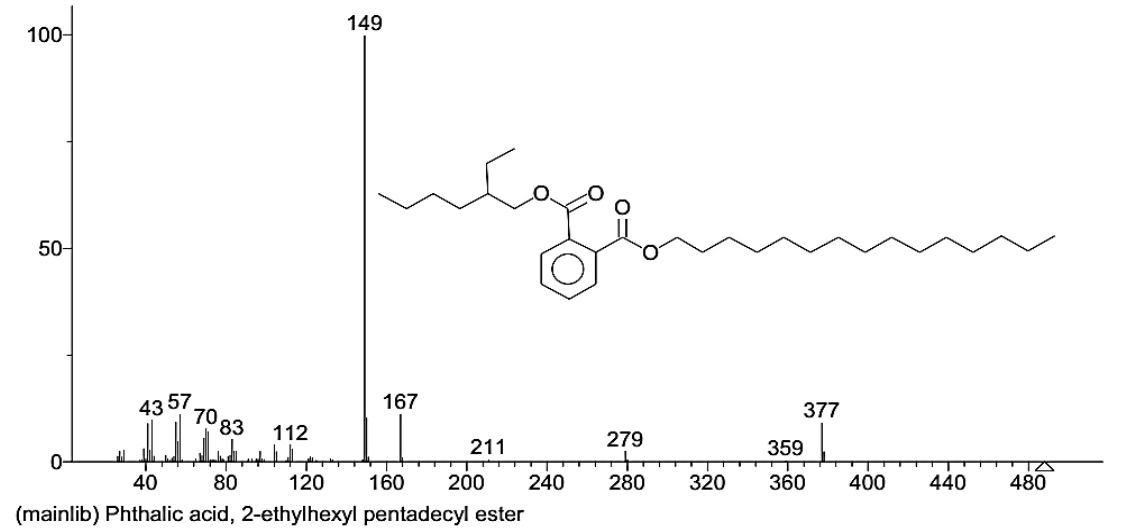


Figure (a). *Phthalic acid, 2-ethylhexyl pentadecyl ester*

Formula: C31H52O4

MW: 488 Exact Mass: 488.38656



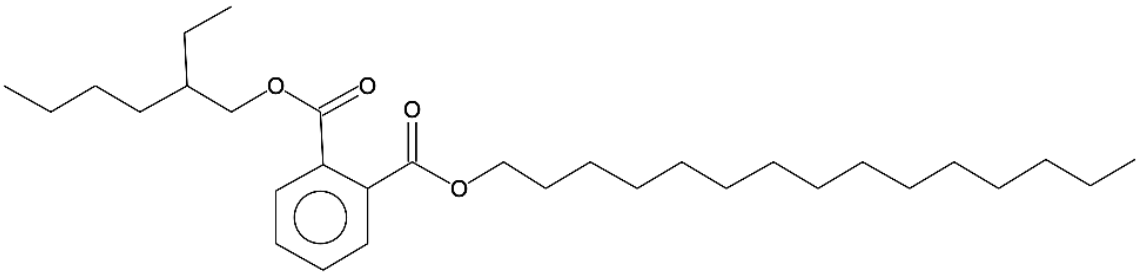
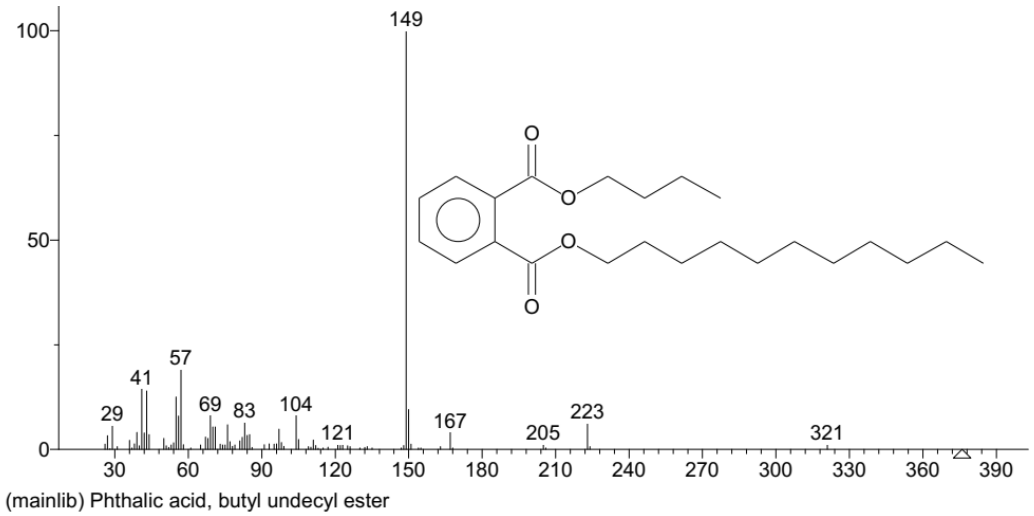


Figure (b)



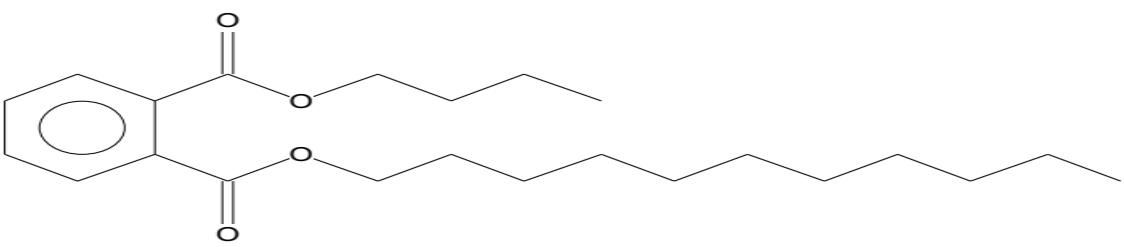
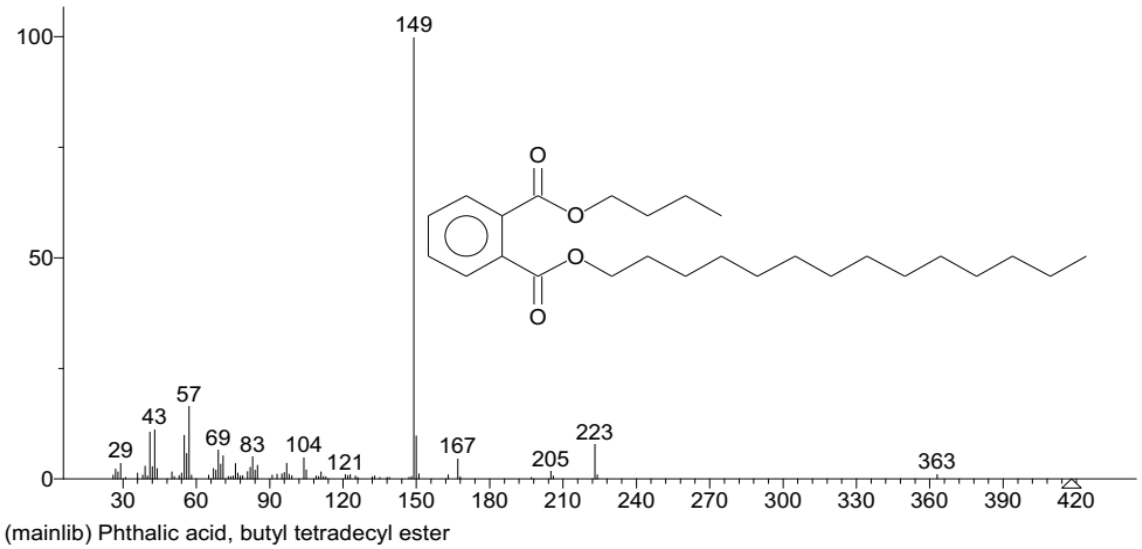


Figure (c). *Phthalic acid, butyl undecyl ester*

Formula: C23H36O4

MW: 376 Exact Mass: 376.26136



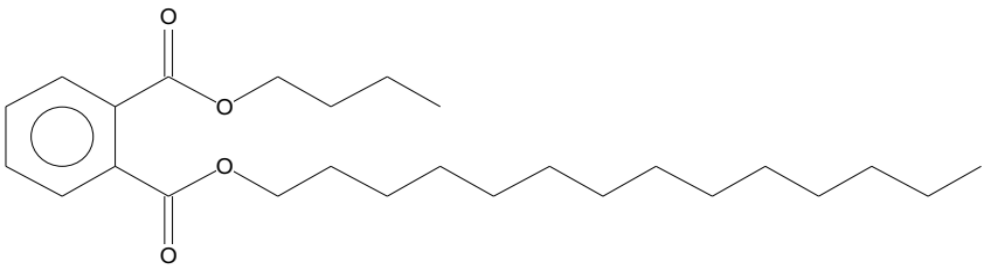
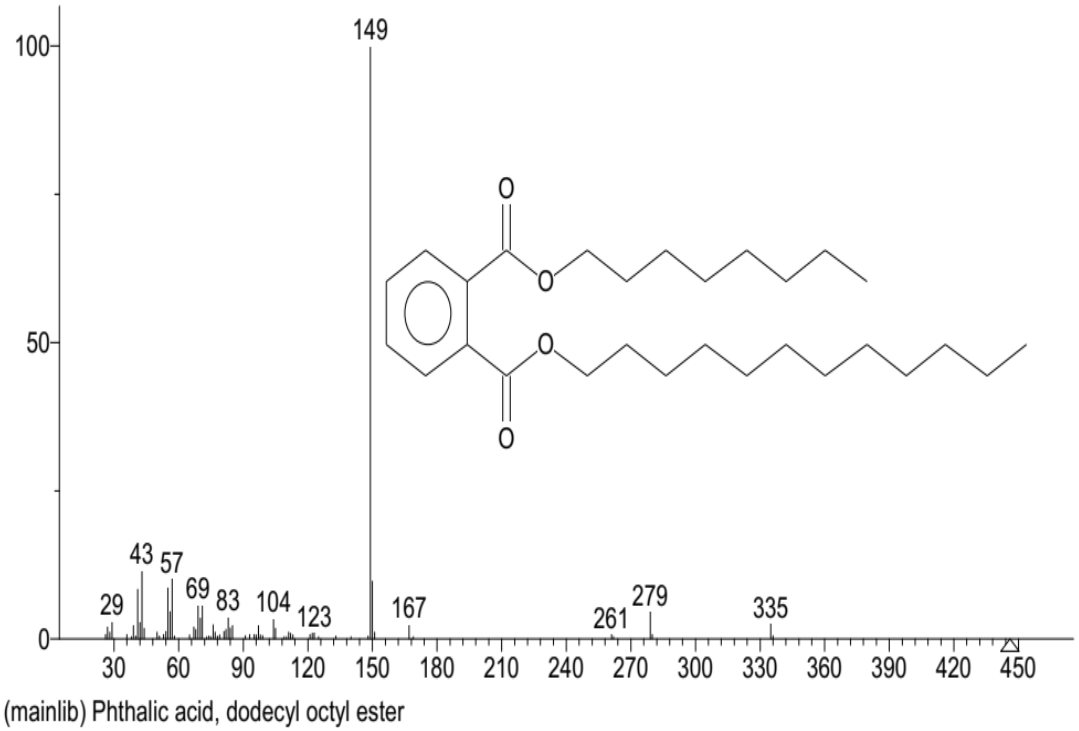


Figure (d). *Phthalic acid, butyl tetradecyl ester*
Formula: C26H42O4
MW: 418 Exact Mass: 418.30831



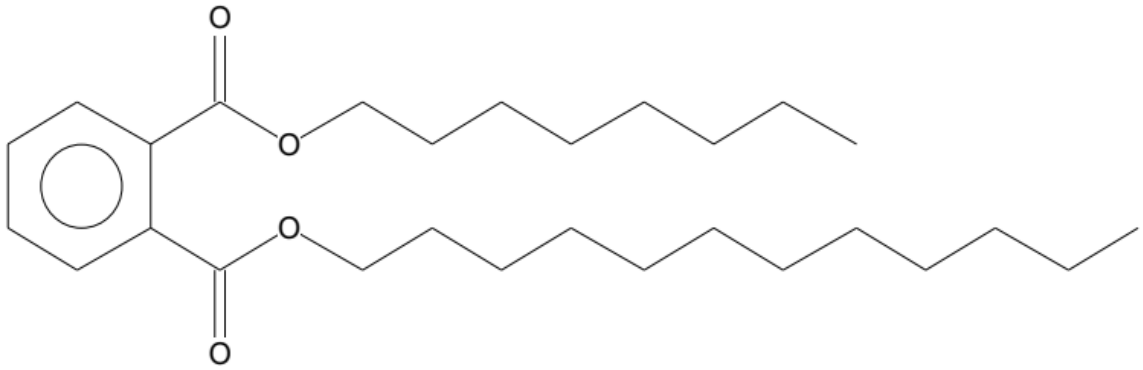
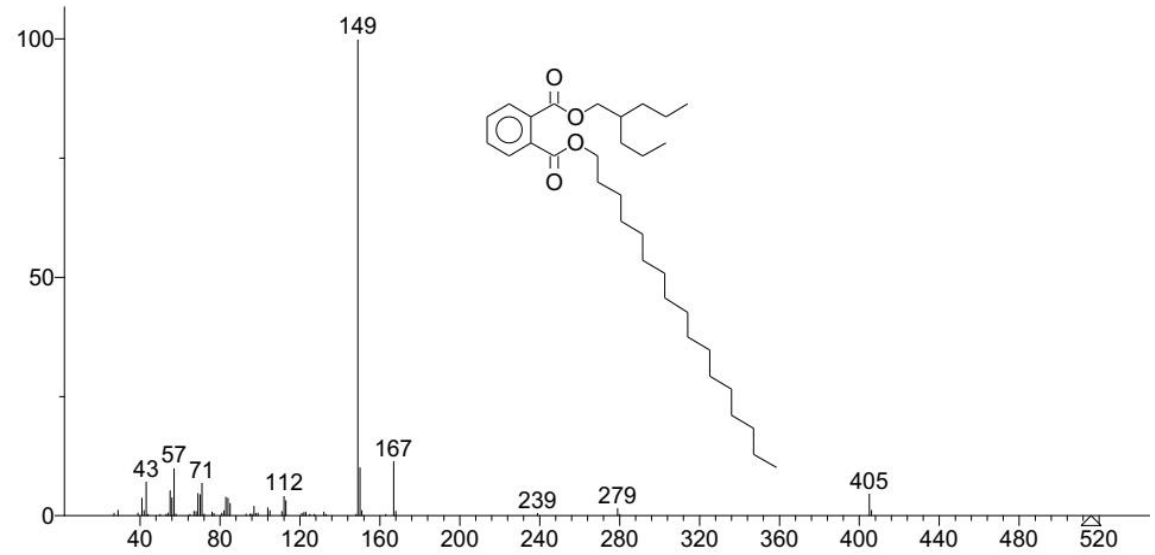
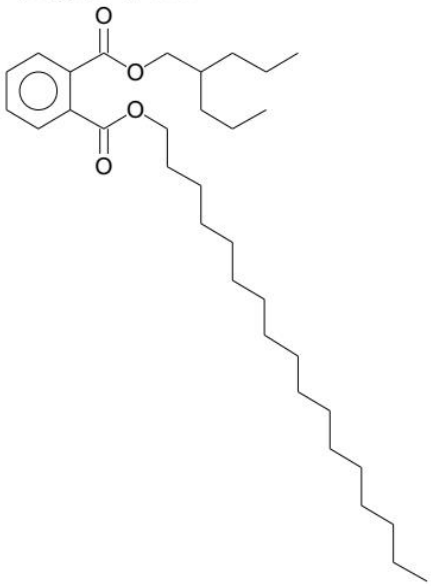


Figure (e). *Phthalic acid, dodecyl octyl ester*
Formula: C28H46O4
MW: 446 Exact Mass: 446.33961

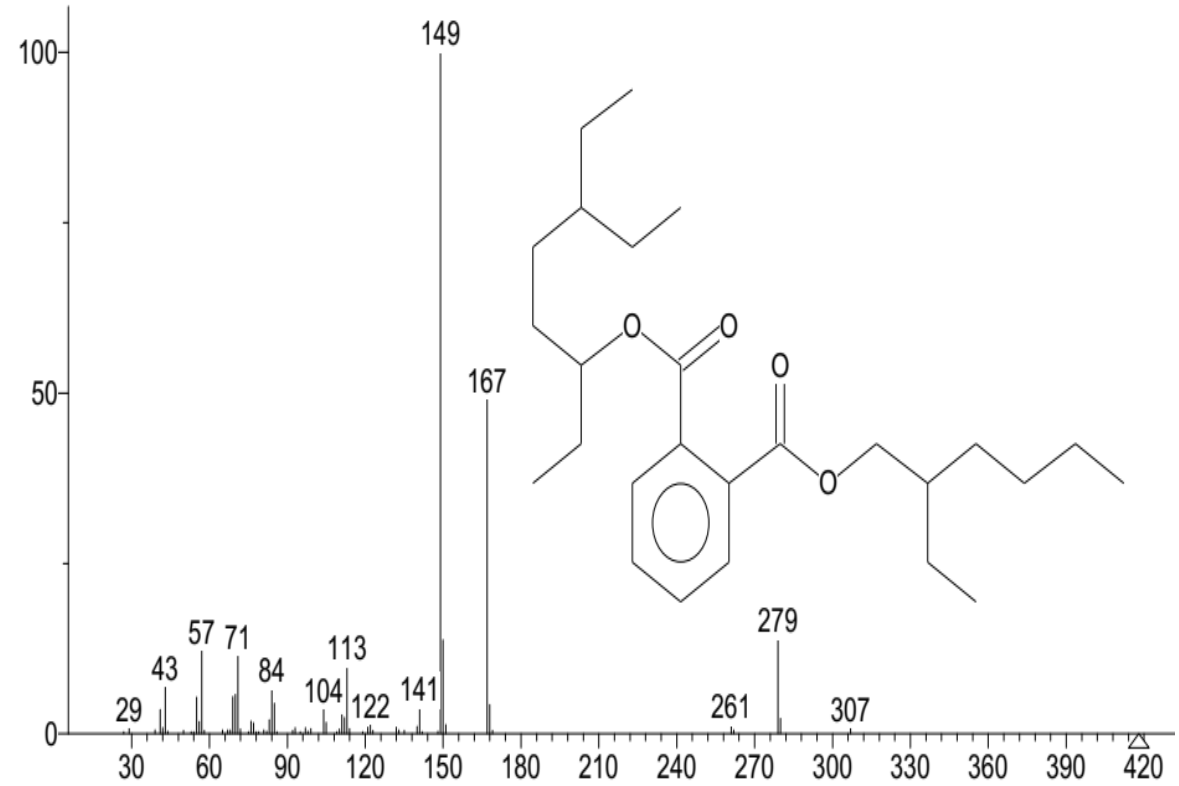


(mainlib) Phthalic acid, heptadecyl 2-propylpentyl ester

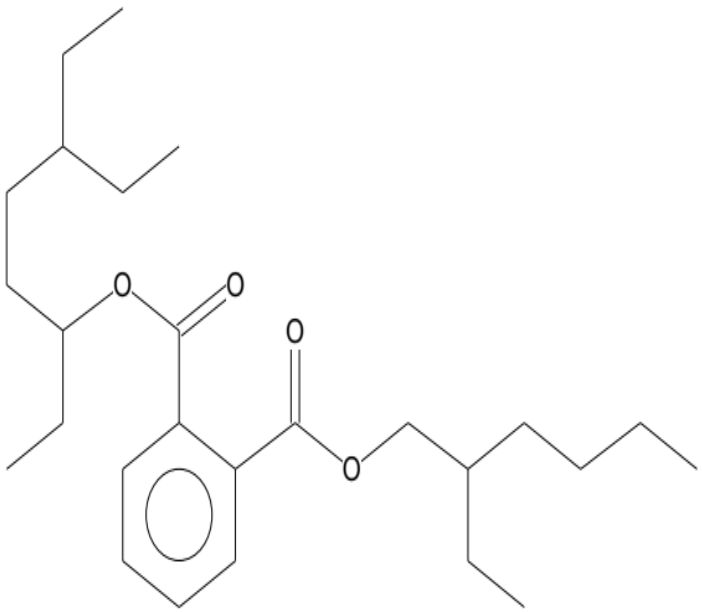


Name: Phthalic acid, heptadecyl 2-propylpentyl ester
Formula: $C_{33}H_{56}O_4$
MW: 516 Exact Mass: 516.417862 NIST#: 377933 ID#: 172419 DB: mainlib

Figure (f)

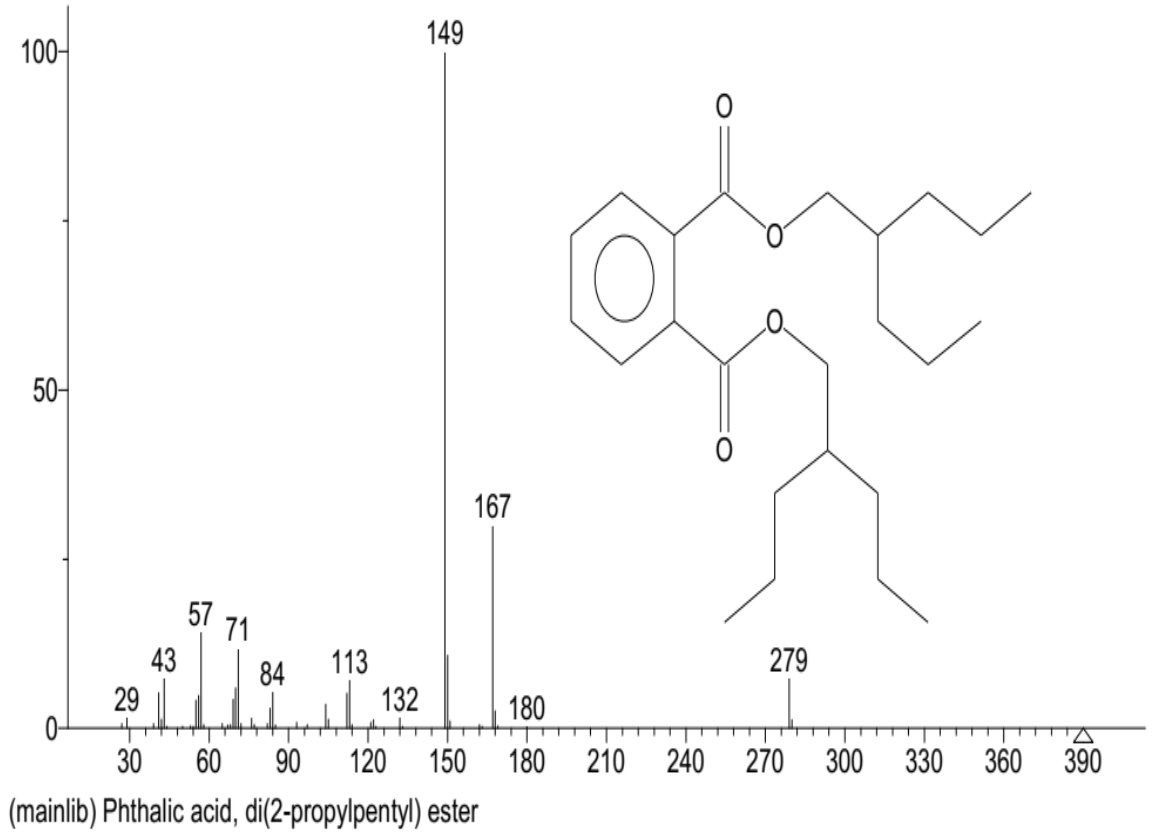


(mainlib) Phthalic acid, 6-ethyloct-3-yl 2-ethylhexyl ester

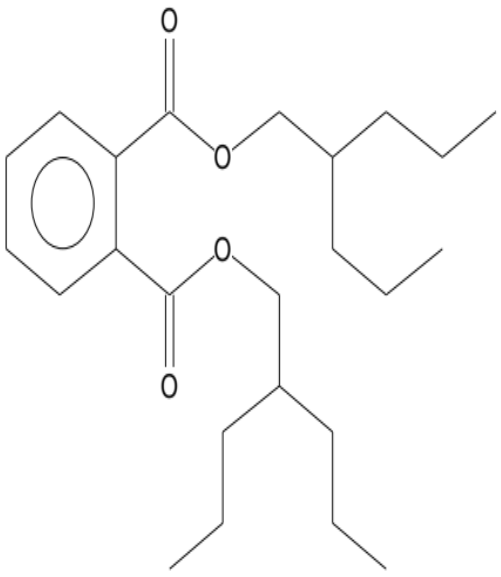


Name: Phthalic acid, 6-ethyloct-3-yl 2-ethylhexyl ester
Formula: $C_{26}H_{42}O_4$
MW: 418 Exact Mass: 418.30831 NIST#: 315538 ID#: 172530 DB: mainlib

Figure (g)

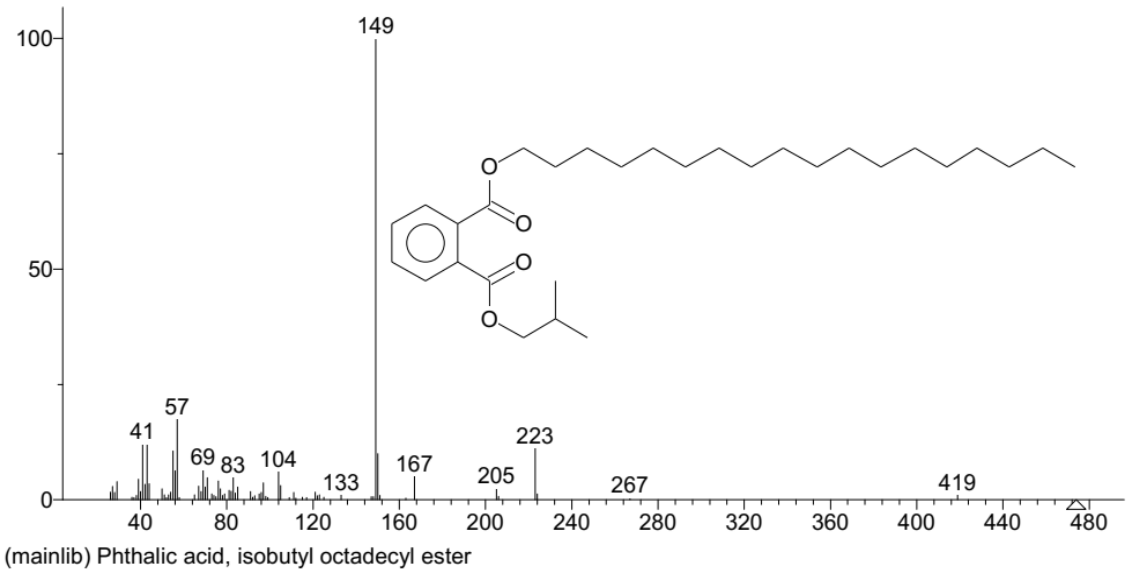


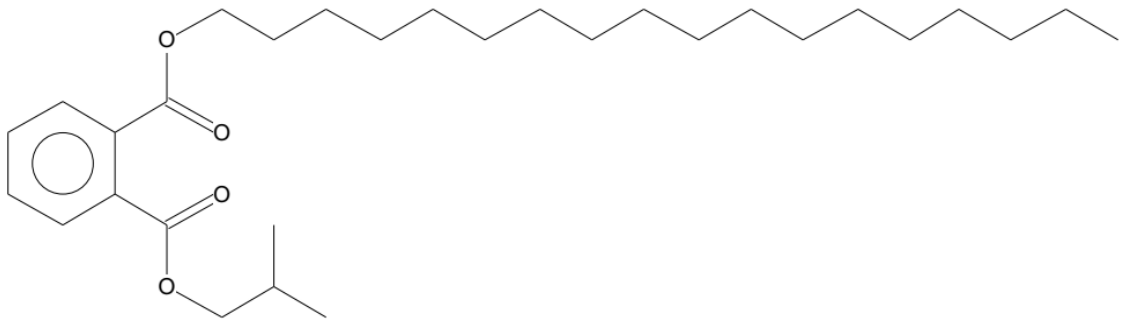
(mainlib) Phthalic acid, di(2-propylpentyl) ester



Name: Phthalic acid, di(2-propylpentyl) ester
Formula: $C_{24}H_{38}O_4$
MW: 390 Exact Mass: 390.27701 NIST#: 377935 ID#: 172420 DB: mainlib

Figure (h)





Name: Phthalic acid, isobutyl octadecyl ester
Formula: $C_{30}H_{50}O_4$
MW: 474 Exact Mass: 474.37091 NIST#: 309061 ID#: 170445 DB: mainlib

Figure (i)

4. Conclusion

The phytochemical screening and GC-MS analysis of *Melastomastrum capitatum* A. & R. Fern. methanol root extract revealed the presence of several bioactive compounds, notably phthalate esters such as phthalic acid, 2-ethylhexyl tetradecyl ester; phthalic acid, butyl undecyl ester; phthalic acid, butyl tetradecyl ester; and phthalic acid, dodecyl octyl ester as well as other bioactive compounds. These compounds, characterized by their long-chain hydrophobic moieties, demonstrate promising anti-brain tumor potential, possibly through mechanisms involving oxidative stress induction, mitochondrial dysfunction, and inhibition of key survival signaling pathways in tumor cells. The presence of these esters supports the therapeutic relevance of *M. capitatum* as a natural source of novel anticancer agents, particularly against aggressive brain tumors such as glioblastoma.

Further pharmacological and toxicological studies are warranted to validate the efficacy and safety of these compounds in targeted brain tumor therapy.

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CONFLICT OF INTERESTS

We have none to declare.

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