**Qualitative phytochemical profile of turmeric (*Curcuma longa* L.) grown in Benin, West Africa.**

**Running title:** Qualitative phytochemical profile of Benin’s Turmeric.

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# Novelty statement

The phytochemical assessment of turmeric products used in Benin is missing in the literature. Therefore, GCMS method was used to assess the qualitative phytochemeical profile of turmeric (*Curcuma longa* L.) grown in Benin, West Africa. Turmeric sourced from Benin has been characterized for first time which provides information about its quality.

# Abstract

*Curcuma longa* L., commonly known as Turmeric, is a versatile herb globally applied in traditional cuisine as spice and involved in different industrial products such as textiles, medicines, confections, and cosmetics. Its diverse applications are attributed to its rich phytochemicals contents. Despite its prevalent use in Beninese bakeries and pastries additionally to as cooking spice, there has been a notable absence of comprehensive compositional analyses specific to the locally cultivated turmeric variant. In this study, the phytochemical composition analysis of turmeric sourced from Benin was conducted by qualitative Gas Chromatography Mass Spectrometry (GCMS). Turmeric rhizomes were obtained from the leading center of cultivating, processing and marketing turmeric products in Benin. After washed with tap water, rhizomes were air dried and ground in fine powder which was used for extraction. The plant extraction was carried out by soxhlet method with n-hexane and obtained oleoresin was used for GCMS analysis. It is found that ar-turmerone (6.32%) and turmerone (2.88%) were identified as the major constituents of *C. longa* L. grown in Benin. These findings suggest that turmeric grown in Benin contains distinctive compounds of *C. longa* L. and consequently could be explore for industrial and pharmaceutical applications. This study underscores the need for further research, specifically focusing on the extraction and quantification of curcumin, a vital bioactive compound of turmeric. Such investigations hold promise for a comprehensive understanding of Benin’s turmeric, facilitating its exploitation in diverse industrial sectors and contributing to scientific knowledge and economic development.

Keywords: Turmeric, GCMS, Phytochemicals, Ar-turmerone, Turmerone.

# INTRODUCTION

Numerous herbs and spices have been utilized for a very long time in traditional remedies. One such perennial herb is turmeric, which is scientifically known as *Curcuma longa* L. in Zingiberaceae family.It is a widespread spice used in domestic cuisine, and its oils and rhizomes play an important role. It is also utilized as a coloring agent for textiles, medicines, confections, and cosmetics when combined with other natural colors (Singh, et al., 2003). The medicinal properties of turmeric extend beyond its culinary use, with applications in AIDS, cancer, dermatitis, and excessive cholesterol management medications (Kuttan, et al., 1985; Ammon & Wahl, 1991; Azuine & Bhide, 1992). The root of turmeric has earned a reputation for its myriad health benefits encompassing antibacterial, antiviral, anti-aging, anti-cancer, anti-Alzheimer's disease, antifungal, antioxidant, and anti-inflammatory qualities (Álvarez, et al., 2016; Hefnawy, et al., 2016; Martinez-Correa, et al., 1017; Singh, et al., 2017; Sornpet, et al., 2017; Wu, et al., 2017; Lu, et al., 2018).

Turmeric diverse applications are attributed to its rich phytochemicals contents with about 235 compounds have been identified from the species, mostly terpenoids and phenolic compounds. These include 22 diarylpentanoids and diarylheptanoids, 8 phenylpropene and other phenolic compounds, 68 monoterpenes, 109 sesquiterpenes, 5 diterpenes, 3 triterpenoids, 4 sterols, 2 alkaloids, and 14 other compounds. Essential oils and curcuminoids, or diarylheptanoids, are the main bioactive components that exhibit a range of bioactivities in both *in vitro* and *in vivo* bioassays. While the composition of turmeric rhizomes' essential oils varies significantly with types and geographical areas, the amount of curcuminoids in the rhizomes varies often depending on sources, locations, and growth conditions. Consequently, there can be a significant variation in the quality of commercial turmeric products. Curcumin, demethoxycurcumin, and bisdemethoxycurcumin have been employed as marker compounds for rhizomes, powders, and extract ("curcumin") products quality control; however, Ar-turmerone, α-turmerone, and β-turmerone can be used to regulate the quality of turmeric oil and oleoresin products. Turmeric products can be verified for authenticity using chromatographic and NMR methods, DNA markers, morphological and anatomical information, GAP, and other available data. (Li, et al., 2011).

As chromatographic technique, the Gas Chromatography Mass Spectrometry (GCMS) which is used for identifying the nonpolar and volatile classes of compound in the extract has emerged as an invaluable technique to delve deeper into botanical wonder and other materials (Dinan, 2006). It has been widely adopted to decipher the phytochemical constituent of turmeric (Ming, et al., 2009; Singh, et al., 2010; Abdel-Shafy, et al., 2020) from which, mostly Ar-turmerone was identified as the major compounds (Shagufta, et al., 2010; Momoh, et al., 2022).

Despite its global recognition, the characterization of turmeric grown in a specific regions remains a compelling area of research. In this regard the present study focuses on the phytochemical composition analysis of turmeric cultivated in the vibrant agricultural landscape of Benin, West Africa. Although turmeric is a staple spice in traditional Beninese cooking, bakeries and pastries, there has been a conspicuous lack of report on the phytoconstituents of the local turmeric variety. Consequently this study endeavors to bridge this knowledge gap through a qualitative GCMS analysis. This investigation holds significant promise for unveiling the unique phytochemical profile of Benin’s turmeric, shedding light on whether it possesses distinctive compounds compared to its counterparts from other regions. The finding from this study may have far-reaching implications in the domains of traditional medicine, pharmaceuticals and culinary arts. Understanding the specific chemical composition of this region variation of turmeric paves the way for enhanced applications in both traditional and modern contexts.

# MATERIAL AND METHOD

# Plant material

Turmeric fresh rhizomes (Figure 1) used in this study were sampled from Songhaї Center at Porto Novo, Benin Republic; the leading center of cultivating, processing and marketing turmeric products in Benin. The plant material was identified by Muhammad Qasim Hayat at Medicinal Plants and Plant Systematic Research Laboratory, Department of Plant Biotechnology, Atta Ur-Rahman School of Applied Biosciences, National University of Sciences & technology, H-12 Sector, Islamabad, Pakistan. After washed with tap water, rhizomes were air dried and ground in fine powder and then used for extraction.

# Plant extract preparation

The extraction was done based on modified method described by (Singh, et al., 2010) using soxhlet apparatus. Plant material and solvent (n-hexane) were in a 1:10 ratio and temperature was set at 55ºC. After 3h, the solvent dropping from extraction chamber to the bottom round flask was clear indicating that the extraction is completed and consequently it was stopped. The obtained extract were concentrated by evaporating total solvent and resulted oleoresin kept at 4 ºC for further utilization.

# GCMS analysis

The qualitative GCMS analysis was performed according to (Singh, et al., 2010) through Shimadzu GCMS QP2020 instrument with column specifications as follows: Shimadzu SH-Rxi-5Sil MS (L=30m, ID=0.25, DF=0.25). Temperature was maintained at 280 ºC for injector, 280 ºC for interphase, 230 ºC for ion source and 150 ºC selective mass detector. The carrier gas was Helium (He) at a flow rate of 1.0mL/min. Oven temperature programmed at 60 ºC for 1 min, then increased from 60 to 185 ºC at the rate of 1.5 ºC/min and held at 185 ºC for 1 min; then again increased from 185 ºC to 275 ºC at the rate of 9 ºC/min and held at 275 ºC for 2 min.

# RESULTS

From the turmeric oleoresin, ninety six compounds were identified by GCMS analysis, six of which were distinctive phytochemicals of turmericNames, molecular formulae and area percentages of distinctive compounds of *Curcuma longa* L. identified from turmeric oleoresin in this study are listed in Table 1 wherea, the total identified compounds are included in Appendix. This report is the first one from turmeric grown in Benin.

# DISCUSSION

These six compounds have already been reported from turmeric in previous works (Ming, et al., 2009; Singh, et al., 2010; Abdel-Shafy, et al., 2020; Shagufta, et al., 2010) and known as distinctive compounds of turmeric.

In this study, Ar-turmerone and Turmerone were the most abundant compounds in the extract, accounting for 6.32% and 2.88%, respectively. Similar results from turmeric were reported by (Abdel-Shafy, et al., 2020) in their study of efficacy and safety of ethanolic *Curcuma longa* L. extract as a treatment for sand tampan ticks in a rabbit model and by (Shagufta, et al., 2010) who studied the chemical analysis of essential oils from turmeric (Curcuma longa) rhizome through GC-MS. Additionally, Ar-turmerone have been identified as the most abundant with peak area of 50.05% on turmeric from Nigeria by (Momoh, et al., 2022) while studying the Phytochemical Screening, Atomic Absorption Spectroscopy, GC-MS and Antibacterial Activities of Turmeric (*Curcuma longa* L.) Rhizome Extracts. Figure 2 is showing the structure of the identified distinctive compounds from turmeric grown in Benin.

According to (Li, et al., 2011), Ar-turmerone, α-turmerone, and β-turmerone can be used to regulate the quality of turmeric oil and oleoresin products. Thus the presence of Ar-turmerone and other distinctive compounds in the Beninese turmeric oleoresin attesting its authenticity.

# CONCLUSION

In this study it is found that along with other identified distinctive compounds, ar-turmerone and turmerone were the abundant constituents in the oleoresin extract of turmeric (*Curcuma longa* L.) sourced from Benin, as found on turmeric from other regions. Therefore, the authenticity for the quality of turmeric grown in Benin is confirmed and could be explored for more applications. Moreover, the extraction and quantification of curcumin from *Curcuma longa* L. cultivated in Benin will give valuable insight on the industrial and pharmaceutical application of this plant.

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**Conflict of interests**

The authors declare that they have no competing interest either financially or personal relationships that could have influenced the writing of this paper.

**Author contribution**

Study concept and design: M.K, MQY and ELW; Acquisition of data: MK; Analysis and interpretation of data: MK and ZZ; Drafting of the manuscript: MK and ZZ; Administrative, technical, and material support: MQY and ELW; Study supervision: MQY

# REFERENCES

Abdel-Shafy, S. et al., 2020. Efficacy and safety of ethanolic Curcuma longa extract as a treatment for sand tampan ticks in a rabbit model. *Veterinary World,* 29 Apr, 13(4), pp. 812-820.

Álvarez, N. M., Ortíz, A. A. & Martínez, O. C., 2016. In vitro antibacterial activity of Curcuma longa (Zingiberaceae) against nosocomial bacteria in Montería, Colombia. *Rev Biol Trop,* 64(3), pp. 1201-1208.

Ammon, H. P. T. & Wahl, M. A., 1991. Pharmacology of Curcuma longa. *Planta Medica,* Volume 57, pp. 1-7.

Azuine, M. A. & Bhide, S. V., 1992. Chemopreventive effect of turmeric against stomach and skin tumors induced by chemical carcinogenesis in Swiss mice. *Nutrition and Cancer,* Volume 17, p. 77–83.

Dinan, L., 2006. Dereplication and Partial Identiﬁcation of Compounds. In: D. S. Satyajit, L. Zahid & I. G. Alexander, eds. *Natural products isolations.* 2nd ed. Totowa(New Jersey): Humana Press, p. 307.

Hefnawy, H., El-Shourbagy, G. & Ramadan, M., 2016. Phenolic extracts of carrot, grape leaf and turmeric powder: antioxidant potential and application in biscuits.. *J. Food Meas. Charact.,* 10(3), pp. 576-583.

Kuttan, R., Bhanumathy, P., Nirmala, K. & George, M. C., 1985. Potential anticancer activity of turmeric (Curcuma longa). *Cancer Letter ,* Volume 29, p. 197–202.

Li, S. et al., 2011. Chemical composition and product quality control of turmeric (Curcuma longa L.). *Pharma. Crops,* Volume 2, p. 28–54.

Lu, P., Inbaraj, B. & Chen, B., 2018. Determination of oral bioavailability of curcuminoid dispersions and nanoemulsions prepared from Curcuma longa Linnaeus. *J. Sci. Food Agric.,* 98(1), pp. 51-63.

Maia, J., Andrade, E. & Zoghbi, M. d. G. B., 2000. Volatile Constituents of the Leaves, Fruits and Flowers of Cashew (Anacardium occidentale L.). *JOURNAL OF FOOD COMPOSITION AND ANALYSIS,* Volume 13, pp. 227-232.

Martinez-Correa, H. et al., 1017. Composition and antimalarial activity of extracts of Curcuma longa L. Obtained by a combination of extraction processes using supercritical CO2, ethanol and water as solvents. *J. Supercrit. Fluids,* Jan, Volume 119, pp. 122-129.

Ming, L. et al., 2009. Quality Assessment of Curcuma longa L. by Gas Chromatography-Mass Spectrometry Fingerprint, Principle Components Analysis and Hierarchical Clustering Analysis. *Bull. Korean Chem. Soc.,* 30(10), pp. 2287-2293.

Momoh, J. O., Manuwa, A. A. & Bankole, Y. O., 2022. Phytochemical Screening, Atomic Absorption Spectroscopy, GC-MS and Antibacterial Activities of Turmeric (Curcuma longa L.) Rhizome Extracts. *Journal of Advances in Microbiology,* 23 July, 22(9), p. 116–131.

Shagufta, N., Saiqa, I., Zahida, P. & Sumera, J., 2010. Chemical Analysis of Essential Oils from Turmeric (Curcuma longa) Rhizome Through GC-MS. *Asian Journal of Chemistry,* April, 22(4), pp. 3153-3158.

Singh, G., Kapoor, I. P., Pandey, S. & Singh, O., 2003. Curcuma longa – chemical, antifungal and antimicrobial investigations of rhizome oil. *Indian Perfumer,* 47(2), p. 173–178.

Singh, G. et al., 2010. Comparative study of chemical composition and antioxidant activity of fresh and dry rhizomes of turmeric (Curcuma longa Linn.). *Food Chem. Toxicol.,* 14 Jan, 48(4), p. 1026–1031.

Singh, N., Gupta, S. & Rathore, V., 2017. Comparative antimicrobial study of ethanolic extract of leaf and rhizome of Curcuma longa Linn.. *Pharmacogn. J.,* 9(2), pp. 208-212..

Sornpet, B., Potha, T., Tragoolpua, Y. & Pringproa, K., 2017. Antiviral activity of five Asian medicinal plant crude extracts against highly pathogenic H5N1 avian influenza virus. *Asian Pac. J. Trop. Med.,* 10(9), pp. 871-876.

Wu, J. et al., 2017. Antifungal activity of 122 kinds of Uighur medicines in vitro. *Acad. J. Second Mil. Med. Univ.,* 38(5), pp. 554-562.



**Figure 1:** Turmeric fresh rhizomes from Benin.



**Figure 2:** Distinctive compounds identified in the oleoresin of turmeric from Benin.

**Table 1:** Distinctive compounds of Curcuma longa L. identified from turmeric grown in Benin

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sr No** | **Compound Name** | **Mol. Formula** | **Mol. Weight** | **Area %** |
| 1 | Ar-turmerone | C15H20O | 216 | 6.32 |
| 2 | Turmerone | C15H22O | 218 | 2.88 |
| 3 | (E)-Atlantone | C15H22O | 218 | 0.64 |
| 4 | (Z)-.alpha.-Atlantone | C15H22O | 218 | - |
| 5 | Caryophyllene oxide | C15H24O | 220 | - |
| 6 | Lanceol, cis | C15H24O | 220 | - |

# Appendix

**Table 2:** All identified compound in the oleoresin of turmeric grown in Benin by GCMS

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Sr No** | **Compound Name** | **Mol. Formula** | **Mol. Weight** | **Area %** |
|  |  |  |  |  |
| 1 | 1-Morpholin-4-yl-4-thioxo-1,3,4,5,6,7-hexahydro-cyclopentapyrimidin-2-one | C11H15N3O2S | 253 | 0.18 |
| 2 | L-Theanine | C7H14N2O3 | 174 | 0.08 |
| 3 | 5-Octen-2-ol, 5-methyl- | C9H18O | 142 | 0.32 |
| 4 | Terephthalic acid, 3-methylpentyl undecyl ester | C25H40O4 | 404 | 0.25 |
| 5 | 4-Piperidinone, 1,2,5-trimethyl-, o-(4-nitrophenyl)oxime | C14H19N3O3 | 277 | 0.10 |
| 6 | 1,1,1,3,5,7,9,11,11,11-Decamethyl-5-(trimethylsiloxy)hexasiloxane | C13H42O6Si7 | 490 | 0.36 |
| 7 | Purine, 2,6-diamino-9-[.beta.-d-ribofuranosyl]-1-oxide | C10H14N6O5 | 298 | 0.12 |
| 8 | Thiophene-2-carboxylic acid, 5-ethylthio-4-formyl- | C8H8O3S2 | 216 | 0.31 |
| 9 | 1-Propanethiol, 3-(9-borabicyclo[3.3.1]non-9-yloxy)- | C11H21BOS | 212 | 0.53 |
| 10 | 10-Heneicosene, 11-phenyl | C27H46 | 370 | - |
| 11 | 5,6:7,8-Diepoxycholestan-3.beta.-ol | C27H44O3 | 416 | 0.06 |
| 12 | Hexacosanoic acid, TMS derivative | C29H60O2Si | 468 | 0.15 |
| 13 | 2-(2',4',4',6',6',8',8'-Heptamethyltetrasiloxan-2'-yloxy)-2,4,4,6,6,8,8,10,10-n | C16H48O10Si9 | 652 | 0.09 |
| 14 | Trichloroacetic acid, 2-tetradecyl ester | C16H29Cl3O2 | 358 | 0.49 |
| 15 | Cholesta-8,24-dien-3-ol, 4-methyl-, (3.beta.,4.alpha.)- | C28H46O | 398 | 0.07 |
| 16 | Benzene, (1,1-dimethyldecyl)- | C18H30 | 246 | 0.20 |
| 17 | Doconexent | C22H32O2 | 328 | 0.19 |
| 18 | Cyclohexene, 1-(3-ethoxy-1-propenyl)-, (Z)- | C11H18O | 166 | 0.11 |
| 19 | Hexane, 1-chloro-5-methyl- | C7H15Cl | 134 | 0.19 |
| 20 | Z,Z,Z-1,4,6,9-Nonadecatetraene | C19H32 | 260 | 0.40 |
| 21 | Toluene-4-sulfonic acid, 7-oxabicyclo[2.2.1]hept-2-ylmethyl ester | C14H18O4S | 282 | 0.29 |
| 22 | Ar-tumerone | C15H20O | 216 | 6.32 |
| 23 | 2-Bromononane | C9H19Br | 206 | 0.52 |
| 24 | Tumerone | C15H22O | 218 | 2.88 |
| 25 | 1,3-Diazabicyclo[3.1.0]hexane | C4H8N2 | 84 | 0.42 |
| 26 | ((5-Isopropyl-2-methylcyclohexyl)sulfonylmethyl)benzene | C17H26O2S | 294 | 0.25 |
| 27 | Perilla alcohol angelate | C15H22O2 | 234 | - |
| 28 | Carbonic acid, butyl 6-chlorohexyl ester | C11H21ClO3 | 236 | 0.62 |
| 29 | 2,5-Octadiene, 3,4,5,6-tetramethyl- | C12H22 | 166 | 0.65 |
| 30 | aR-Turmerone | C15H20O | 216 | 0.40 |
| 31 | (E)-Atlantone | C15H22O | 218 | 0.64 |
| 32 | (Z)-.alpha.-Atlantone | C15H22O | 218 | - |
| 33 | cis-Z-.alpha.-Bisabolene epoxide | C15H24O | 220 | 0.58 |
| 34 | Tricyclo[4.2.2.0(2,5)]deca-7,9-diene-7,8-dicarboxylic acid, 3-cyano-, dimet | C15H15NO4 | 273 | 0.10 |
| 35 | 2(1H)-Naphthalenone, 4a,5,8,8a-tetrahydro-4,4a-dimethyl-, trans- | C12H16O | 176 | 0.57 |
| 36 | 3,6-Undecandione | C11H20O2 | 184 | 0.56 |
| 37 | 2-tert-Butyl-4,6-dinitrophenyl trifluoroacetate | C12H11F3N2O6 | 336 | 0.23 |
| 38 | Carbonic acid, but-3-yn-1-yl octyl ester | C13H22O3 | 226 | 0.37 |
| 39 | 3-Methyl-2-butenoic acid, 3-phenylpropyl ester | C14H18O2 | 218 | 0.42 |
| 40 | Propanoic acid, 2-methyl-, decyl ester | C14H28O2 | 228 | 0.28 |
| 41 | Dichloroacetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl | C12H16Cl2O2 | 262 | 0.09 |
| 42 | 1,1':2',1''-Tercyclohexane | C18H32 | 248 | 0.39 |
| 43 | 4H-1,2,4-triazole-3-thiol, 5-methyl-4-[(3-nitro-2-pyridinyl)amino]- | C8H8N6O2S | 252 | 0.18 |
| 44 | 19-Norethindrone, O-methyloxime | C21H29NO2 | 327 | 0.06 |
| 45 | 3-Oxabicyclo[4.1.0]heptane-7-carboxamide, 6-methyl-N-(1-naphthyl)- | C18H19NO2 | 281 | 0.09 |
| 46 | Sorbitol | C6H14O6 | 182 | 0.06 |
| 47 | Nonane, 1-bromo- | C9H19Br | 206 | 0.16 |
| 48 | Nonane, 5-butyl- | C13H28 | 184 | 0.13 |
| 49 | 4-Hexenoic acid, 6-hydroxy-4-methyl-, methyl ester, (E)- | C8H14O3 | 158 | 0.09 |
| 50 | Hydrazine, N-(chloro)(nitro)methylene)-N'-(4-nitrophenyl)- | C7H5ClN4O4 | 244 | 0.16 |
| 51 | 13-[(2,6-Dimethylphenylamino)methyl]tricyclo [8.2. 2.24,7]hexadeca-1(13),4,6,10(14),11,15-hexaen-5-ol | C25H27NO | 357 | 0.09 |
| 52 | Caryophyllene oxide | C15H24O | 220 | - |
| 53 | Propionitrile, 3-[1-[4-[1-(2-cyanoethoxy)cyclohexyl]buta-1,3-diynyl]cyclohexyloxy] | C22H28N2O2 | 352 | 0.17 |
| 54 | Cyclopentanol, 3-methyl-2-(2-pentenyl)- | C11H20O | 168 | 0.25 |
| 55 | 2,3-O-Benzal-d-mannosan | C13H14O5 | 250 | 0.19 |
| 56 | Di-n-octyl phthalate | C24H38O4 | 390 | 14.19 |
| 57 | Propanamide, N-(3-methoxyphenyl) | C12H17NO2 | 207 | 0.22 |
| 58 | 4H,5H-Pyrano[4,3-d]-1,3-dioxin, tetrahydro-8a-methyl- | C8H14O3 | 158 | 0.15 |
| 59 | Lanceol, cis | C15H24O | 220 | - |
| 60 | Cycloheptanone, 2-methyl- | C8H14O | 126 | 0.07 |
| 61 | Bicyclo[2.2.1]heptane-1-carboxylic acid, 4,7,7-trimethyl-3-oxo-2-oxa-, (2,4-difluorophenyl)amide | C16H17F2NO3 | 309 | 0.07 |
| 62 | 2-Oxotetrahydropyranyl-6-acetic acid, methyl ester | C8H12O4 | 172 | 0.07 |
| 63 | Oxazolidin-2-one, 3-tert-butyl-5-phenoxymethyl- | C14H19NO3 | 249 | 0.16 |
| 64 | Pyridine, 2-fluoro-5-iodo- | C5H3FIN | 223 | 0.10 |
| 65 | cis-(.+/-.)-4-Methylaminorex | C10H12N2O | 176 | 0.14 |
| 66 | 5-Hexen-1-ol | C6H12O | 100 | 0.16 |
| 67 | 3-(Octane-1-sulfinyl)propanamide | C11H23NO2S | 233 | 0.13 |
| 68 | 4-Heptenal, (E)- | C7H12O | 112 | 0.06 |
| 69 | 3-Nonenoic acid | C9H16O2 | 156 | 0.14 |
| 70 | Pentadioic acid, dihydrazide, N2,N2'-bis(2-furfurylideno)- | C15H16N4O4 | 316 | 0.08 |
| 71 | Thiocyanic acid, 5-amino-3-methyl-4-isoxazolyl ester | C5H5N3OS | 155 | 0.09 |
| 72 | Geldaramycin | C29H40N2O9 | 560 | - |
| 73 | 5-[(5-Chlorothiophen-2-yl)carbonyl]-2-N-isopropyl-1,3-thiazole-2,4-diamine | C11H12ClN3OS2 | 301 | 0.09 |
| 74 | (2-Benzyl-benzoimidazol-1-yl)-piperidin-1-yl-methanone | C20H21N3O | 319 | 0.07 |
| 75 | 2-Myristynoyl-glycinamide | C16H28N2O2 | 280 | 0.14 |
| 76 | trans-4,5-Epoxynonane | C9H18O | 142 | 0.15 |
| 77 | 6-(4-Chlorophenyl)-5-methyl-4,5-dihydro-3(2H)-pyridazinone, TMS derivative | C14H19ClN2OSi | 294 | 0.10 |
| 78 | Piperidine, 1-(5-aminopentyl)-2-ethyl- | C12H26N2 | 198 | 0.33 |
| 79 | Propanal, 2-methyl-, (2,4-dinitrophenyl)hydrazone | C10H12N4O4 | 252 | 0.13 |
| 80 | 1-Propanamine, N-nitro- | C3H8N2O2 | 104 | 0.09 |
| 81 | Benzene, 1,2,3,5-tetramethyl-4,6-dinitro- | C10H12N2O4 | 224 | 0.25 |
| 82 | n-Pentane, 2-cyclohexyl-5-[1-cycloazapropyl]- | C13H25N | 195 | 0.12 |
| 83 | 2,5-cyclohexadien-1-one, 4-[[4-(diethylamino)-2-methylphenyl]imino]-2-methyl-6-[[methyl(4-nitrophenyl)amino]methyl] | C26H30N4O3 | 446 | 0.14 |
| 84 | Propionic acid, 3-tetrazol-1-yl- | C4H6N4O2 | 142 | 0.07 |
| 85 | Sarpagan-17-ol, 16-[(acetyloxy)methyl]-, acetate (ester) | C24H28N2O4 | 408 | 0.12 |
| 86 | 5-[4-(Dimethylamino)cinnamoyl]acenaphthene | C23H21NO | 327 | 0.13 |
| 87 | 2-Propyl-5-oxohexanoic acid | C9H16O3 | 172 | 0.14 |
| 88 | Myrtenyl tiglate | C15H22O2 | 234 | - |
| 89 | 1,2-Bis(trimethylsilyl)benzene | C12H22Si2 | 222 | 0.10 |
| 90 | 1,3,5-Triazine-2,4,6(1H,3H,5H)-trione, 1,3,5-tri-2-propenyl- | C12H15N3O3 | 249 | 0.03 |
| 91 | Cholestan-16,22-epoxy-26-ol-3-one ethyl ether | C29H48O3 | 444 | - |
| 92 | Spirostan-3,27-diol, (3.alpha.) | C27H44O4 | 432 | - |
| 93 | Brefeldin A | C16H24O4 | 280 | 0.08 |
| 94 | 4Beta,5-epoxy-5beta-cholestan-3-one | C27H44O2 | 400 | - |
| 95 | Isoindole-1,3(2H)-dione, 2-[2-(5-amino-1,2,4-triazol-3-yl)ethyl]- | C12H11N5O2 | 257 | 0.22 |
| 96 | 1-Amino-2-(dimethylamino)-4-hydroxyanthracene-9,10-dione | C16H14N2O3 | 282 | 0.22 |