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**ORIGINAL ARTICLE** **OPEN ACCESS**

# Phytocompound identification from *Cuscuta reflexa*, *Foeniculum vulgare* and *Tinospora cordifolia* using gas chromatography-mass spectrometry and their efficiency on removal of metal toxicity by an *In Silico* approach

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**ABSTRACT**
*Biological approaches that use the plants for silver nanoparticles provide enhanced platforms for nanoparticle synthesis as they are free from toxic chemicals and additionally provide natural capping agents. Nowadays, the use of plant extracts has also reduced the expenditure of the microorganism isolation and also the culture media enhancing the expenditure, competitive possibility above nanoparticles synthesis by the microorganism. Synthesis of nanoparticles using plant extracts are considered as one of the most adopted methods of green and eco-friendly production of nanoparticles where it also has a special advantageous application that the plants are widely distributed, easily available, much safer to handle and act as a source of several metabolites. The present study aims to find the presence of phytochemicals in the selected plants such as methanolic extracts of Cuscuta reflexa leaves Foeniculum vulgare stem and Tinospora cordifolia fruits and also find the docking analysis of these plants by using suitable binders. The result proves that the plant extracts contain various important bioactive components and this may be the results of its various activities. The docking analysis also proves its efficiency.*
***Keywords:*** *Cuscuta reflexa, Foeniculum vulgare, Tinospora cordifolia, GC-MS, In silico, Metal toxicity*

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## INTRODUCTION

Almost 70 % of the industrial wastes are produced by developing countries and they are disposed of untreatably into the nearby water bodies where they contaminate the existing water sources. Every year, the world generates around 400 billion tons of industrial wastes, mostly in the form of different chemicals that are discharged either directly or indirectly into the aquatic environment without any adequate treatment to remove their harmful effects [1]. The quality of the groundwater can be determined by assessing its physical, chemical and bacteriological properties of it. These parameters of the groundwater may be varied and it is greatly influenced by natural processes such as geological formations and anthropogenic activities. Industrial waste and municipal solid waste have emerged as one of the leading causes of pollution of surface and groundwater [2].

Many researchers have been indulged in the various studies that concentrate on assessing the groundwater quality and pollution sources influenced by industrial and natural processesworldwide. The principles governing the chemical characteristics of groundwater and the influence of anthropogenic activities are well documented in many parts of India [3]. Occasionally the nanoparticles synthesis from the plant sources and its extracts can be advantageous over other biological synthesis processes [4], which involve the very complex procedures of maintaining microbial cultures [4]. Synthesis of nanoparticles with certain microbes such as the using fungi like *Fusarium oxysporum* [5], *Penicillium* sp. [6] and using some bacteria such as *Bacillus subtilis* etc., [7] has now come into the field with higher efficiencies.

Synthesis of nanoparticles using plant extracts are considered as one of the most adopted methods of green and eco-friendly production of nanoparticles where it also has a special advantageous application that the plants are widely distributed, easily available, much safer to handle and act as a source of several metabolites [8] The aim of the present study is to identify the Phyto-based nanomaterials using three

different plants namely, *Cuscuta reflexa.* Roxb*, Foeniculum vulgare.* Mill and *Tinospora cordifolia* (Thunb.) Miers of recent advances in tap water and wastewater treatment processes is provided. The activity of these plants may be the presence of secondary metabolites. This study especially concentrates on the identification of the phytocompounds present in the extract as well as the molecular docking analysis.

## MATERIAL AND METHODS

The *C. reflexa* leaves were collected fresh from the foothills of the Nilgiri region and the *F. vulgare* stem and *T. cordifolia* fruits were collected from the Yercaud regions of the Salem district. The collected parts of the various plants said above was shade dried and powdered to contribute to 57 g, 46.4 g and 37.8 g of the plant extracts before shade drying.

## SAMPLE PREPARATION

The 10 g of each plant (*C. reflexa, F. vulgare* and *T. cordifolia*) were taken and added to 100 ml of Milli Q water and then boiled at a temperature of 80°C for approximately 45 minutes and the obtained mixture was filtered using Whatman Filter paper No. 1 (HiMedia Labs Ltd.) separately to give the aqueous extracts and then were stored at 4°C for further use.

## GAS CHROMATOGRAPHY-MASS SPECTROMETRY PROTOCOL

Gas chromatography-mass spectrometry (GC-MS) allows users to selections cleaved by electron ionization (EI), and then cleave precursor ions *via* collision-induced dissociation (CID), this enables a detailed analysis of partial structures. A production scan can be used to easily discriminate between structural isomers and positional isomers, which are hard to identify from EI mass spectra obtained with a single GC-MS system. That makes production scans ideal for predicting partial structures. Using this technique the samples were prepared according to the manual provided and loaded in the system. The analysis of the samples was done by running the multiple sample analysis parameters and the processed data was obtained and stored for further clarifications. The single sample analysis and the multiple sample analysis chromatographs were obtained.

## DOCKINTG ANALYSIS

Molecular docking study plays an important role in the field of food, drug pollution treatment and also to find out the binding affinity between the compounds. This study was designed to find the binding efficiency of the derived phytochemical compound from the GC-MS results obtained with the CusBA heavy-metal efflux complex from *Escherichia coli.* The molecular docking results show that the phthalic acid from the phytochemical derived from the three different plant extracts have been showing better binding activity with the heavy metal complex, which indirectly depicts that the plant extracts have an efficient ability to deteriorate or remove heavy metal toxicants from the solvent effluents and also the phytochemical compoundis satisfying Lipinski's rule of 5 and ADMET properties, to be an inhibitor.

## RESULT AND DISCUSSION

Now-a-days, GC-MS studies have been highly used for the analysis of phytocompounds present in the different extracts of plants [9-12] show that there is a presence of the flavonoid compounds namely indigotin, indirubin, tryptanthrin, isatin, rutin, lupeol in the *Wrightia tinctoria* leaf extracts using GC-MS studies. Whereas, Rangaswami and Rao [13] initially showed that there is a presence of the terpene compounds α-amyrin and β-amyrin respectively in the leaf, seed, bark, mature and immature seed pods extracts of the leaf extracts ofthe plant.

Similarly, later on, Pritam and Sanjay [14] reported that there was another terpene compound lupeol in the leaf, seed, bark, stem extracts of the plant on GC-MS analysis. Similarly, the study reported by Selvaraj and Prassana [15] show that the analysis of methanolic stem extract of *T. cordifolia* has eleven compounds, which including 2,4-bis**(**1,1- dimethylethyl**)**, hepta-decenal, 3,7,11,15-tetramethyl-2-hexa-decen-1-ol, hepta-decyl- trifluoro-acetate, phenol, trifluoro-acetoxy hexadecane, 9-eicosene, **(**e**)**-$C_{20}H_{40}$ 7 24.47 octadecane, 3-ethyl-5-**(**2-ethylbutyl**)**, di-n-decylsulfone, hexamethyl-cyclotrisiloxane cyclohexane,1,1'-**(**2-tridecyl-1,3-propanediyl**)**bis and 1,4-didecyl-cyclohexane.

In concordance with this, the present study has reported that the chloroform extracts of the plant, *C. reflexa* leaves, *F. vulgare* stem and *T. cordifolia* fruits show the following observations as shown in the Table 1 compound were identified by GC-MS analysis of the *C. reflexa* leaves are shown in Figure 1. The compounds are cyclooctasiloxane, hexadecanoic acid, phthalic acid, 9-octadecenoic acid, heptadecanoic acid, methyl 10-oxohexadecanoate, eicosa methyl cyclodeca siloxan, eicosanoicacid, cyclodecasiloxane, tetracosamethyl-cyclododecas, cyclodecasiloxane and tetracosamethyl-cyclododecas.

Figure 2 showed the compounds were identified by GC-MS analysis in *F. vulgare* stem. The compounds are hexadecanoic acid, phthalic acid, ethyl linoleate, 9-octadecenoic acid, ethyloleate, heptadecanoic acid, methyl 10-oxohexadecanoate, eicosamethyl cyclodecasiloxan,eicosanoic acid and iron.

The results of the GC-MS analysis of *T. cordifolia* fruits are shown in Figure 3. Several different

phytoconstituents are identified in the sample 3 such as hexadecanoic acid, phthalic acid, ethyl linoleate, 9-octadecenoic acid, 6-tridecenoic acid, ethyl oleate, di-(9- octadecenoyl)-glycerol, 2-cyclopentene-1-tridecanoic acid, heptadecanoic acid, 1H-purin-6- amine, methyl 10-oxohexadecanoate and eicosanoic acid.

The Phthalic is thought to originate from lignin-type organic matter **(**phenols**)** which is converted to aromatic diacids by microbial action. Phthalic acid is believed to get subjected to anaerobic treatment and is mineralized by anaerobic lake sediment. From the compound structure, the results of the present study depict that this compound is an aromatic dicarboxylic acid, with the molecular formula $C_6H_4$**(**COOH**)**$_2$. In the present study, it is clear that all the three plant extracts have shown the presence of Phthalic acid through GC-MS analysis and it is clear that this compound would serve as a strong environmental waste deterioration when added in proper concentration to the water bodies. The same is later depicted from the Docking studies.

**Table 1 Bioactive compound identified using GC-MS**

| Figure Numbers | Details |
|---|---|
| **Figure 1** | # RT Peak Name Res Type Area Amount R. Match<br>1. 12.566 Cyclooctasiloxane, hexadecam TIC 297052 0.440 768<br>2. 19.484 Hexadecanoic acid, methyl es TIC 2.480e+6 3.678 85<br>3. 20.341 Phthalic acid, butyl hexyl e TIC 1.133e+6 1.681 957<br>4. 23.497 9-Octadecenoic acid **(**Z**)**-, me TIC 1.092e+7 16.191 841<br>5. 23.633 9-Octadecenoic acid **(**Z**)**-, me TIC 2.448e+6 3.630 826<br>6. 24.052 Octadecanoic acid, methyl es TIC 1.110e+7 16.460 842<br>7. 24.861 Ethyl Oleate TIC 8.831e+6 13.095 816<br>8. 25.240 Hexadecanoic acid, butyl est TIC 2.626e+6 3.894 742<br>9. 25.394 Heptadecanoic acid, 15-methy TIC 6.296e+6 9.336 728<br>10. 27.513 Methyl 10-oxohexadecanoate TIC 1.418e+6 2.102 749<br>11. 27.650 Eicosamethylcyclodecasiloxan TIC 971186 1.440 839<br>12. 27.903 Eicosanoic acid, methyl este TIC 1.080e+6 1.602 853<br>13. 28.919 Octadecanoic acid, butyl est TIC 1.314e+6 1.949 767<br>14. 29.976 Cyclodecasiloxane, eicosamet TIC 1.112e+6 1.650 828<br>15. 36.249 Tetracosamethyl-cyclododecas TIC 1.385e+6 2.054 864<br>16. 38.885 Cyclodecasiloxane, eicosamet TIC 2.103e+6 3.119 761<br>17. 41.073 Tetracosamethyl-cyclododecas TIC 2.068e+6 3.067 821<br>18. 43.071 Tetracosamethyl-cyclododecas TIC 2.200e+6 3.262 819 |
| **Figure 2** | # RT Peak Name Res Type Area Amount R. Match<br>1 19.482 Hexadecanoic acid, methyl es TIC 3.804e+6 3.930 861<br>2 20.336 Phthalic acid, butyl hexyl e TIC 1.202e+6 1.242 945<br>3 21.116 Hexadecanoic acid, ethyl est TIC 1.936e+6 2.000 713<br>4 23.357 Ethyl linoleate TIC 894070 0.924 864<br>5 23.502 9-Octadecenoic acid **(**Z**)**-, me TIC 1.634e+7 16.877 850<br>6 23.636 9-Octadecenoic acid **(**Z**)**-, me TIC 1.593e+6 1.646 825<br>7 24.057 Octadecanoic acid, methyl es TIC 1.239e+7 12.802 844<br>8 24.870 Ethyl Oleate TIC 1.671e+7 17.263 807<br>9 25.245 Hexadecanoic acid, butyl est TIC 6.430e+6 6.643 762<br>10 25.400 Heptadecanoic acid, 15-methy TIC 9.663e+6 9.983 741<br>11 27.512 Methyl 10-oxohexadecanoate TIC 1.095e+6 1.132 747<br>12 27.640 Eicosamethylcyclodecasiloxan TIC 1.839e+6 1.900 781<br>13 27.906 Eicosanoic acid, methyl este TIC 1.165e+6 1.204 852<br>14 28.924 Octadecanoic acid, butyl est TIC 3.472e+6 3.588 776<br>15 29.974 Eicosamethylcyclodecasiloxan TIC 2.405e+6 2.485 725<br>20 43.063 Iron, monocarbonyl-**(**1,3-buta TIC 3.126e+6 3.229 725 |

**Figure 3**

# RT Peak Name Res Type Area Amount R. Match
2 19.490 Hexadecanoic acid, methyl es TIC 4.185e+6 4.007 859
3 20.350 Phthalic acid, butyl hexyl e TIC 303223 0.290 958
5 21.118 Hexadecanoic acid, ethyl est TIC 3.424e+6 3.279 731
6 23.358 Ethyl linoleate TIC 570360 0.546 850
7 23.506 9-Octadecenoic acid **(**Z**)**-, me TIC 2.082e+7 19.933 843
8 23.637 9-Octadecenoic acid **(**Z**)**-, me TIC 3.464e+6 3.317 837
9 24.061 Octadecanoic acid, methyl es TIC 1.668e+7 15.975 851
10 24.740 6-Tridecenoic acid, 13-**(**2-cy TIC 1.122e+6 1.074 868
11 24.875 Ethyl Oleate TIC 2.550e+7 24.420 819
12 24.994 DI-**(**9-OCTADECENOYL**)**-GLYCEROL TIC 63788 0.061 789
13 25.253 2-Cyclopentene-1-tridecanoic TIC 1.869e+6 1.790 793
14 25.405 Heptadecanoic acid, 15-methy TIC 1.688e+7 16.160 739
16 27.082 1H-Purin-6-amine, [**(**2-fluoro TIC 583026 0.558 743
17 27.510 Methyl 10-oxohexadecanoate TIC 2.705e+6 2.590 726
18 27.904 Eicosanoic acid, methyl este TIC 1.588e+6 1.520 867

## Plot 1. 10-22-201912-49-04 pm.sms - 10/22/2019 12:49 PM

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| Tangent %: | 10 |
| Peak Size Reject (counts): | 2000 |
| Smoothing: | None |
| Spike Threshold Factor: | None |
| Noise: | Peak to Peak |

| | Retention Time | Area | % of Total | Signal/Noise | Scan Description |
|---|---|---|---|---|---|
| 1. | 10.002 | 501180 | 0.743 | 35 | Merged |
| 2. | 10.184 | 3.037e+6 | 4.504 | 48 | Merged |
| 3. | 10.409 | 1.827e+6 | 2.710 | 43 | Merged |
| 4. | 12.566 | 297052 | 0.440 | 20 | Merged |
| 5. | 19.484 | 2.480e+6 | 3.678 | 122 | Merged |
| 6. | 20.341 | 1.133e+6 | 1.681 | 45 | Merged |
| 7. | 21.115 | 1.205e+6 | 1.786 | 47 | Merged |
| 8. | 23.497 | 1.092e+7 | 16.191 | 298 | Merged |
| 9. | 23.633 | 2.448e+6 | 3.630 | 35 | Merged |
| 10. | 24.052 | 1.110e+7 | 16.460 | 145 | Merged |
| 11. | 24.861 | 8.831e+6 | 13.095 | 134 | Merged |
| 12. | 25.240 | 2.626e+6 | 3.894 | 42 | Merged |
| 13. | 25.394 | 6.296e+6 | 9.336 | 143 | Merged |
| 14. | 27.513 | 1.418e+6 | 2.102 | 20 | Merged |
| 15. | 27.650 | 971186 | 1.440 | 14 | Merged |
| 16. | 27.903 | 1.080e+6 | 1.602 | 18 | Merged |
| 17. | 28.919 | 1.314e+6 | 1.949 | 33 | Merged |
| 18. | 29.976 | 1.112e+6 | 1.650 | 27 | Merged |
| 19. | 32.472 | 1.085e+6 | 1.609 | 25 | Merged |
| 20. | 36.249 | 1.385e+6 | 2.054 | 21 | Merged |
| 21. | 38.885 | 2.103e+6 | 3.119 | 23 | Merged |
| 22. | 41.073 | 2.068e+6 | 3.067 | 23 | Merged |
| 23. | 43.071 | 2.200e+6 | 3.262 | 18 | Merged |

**Cont….**

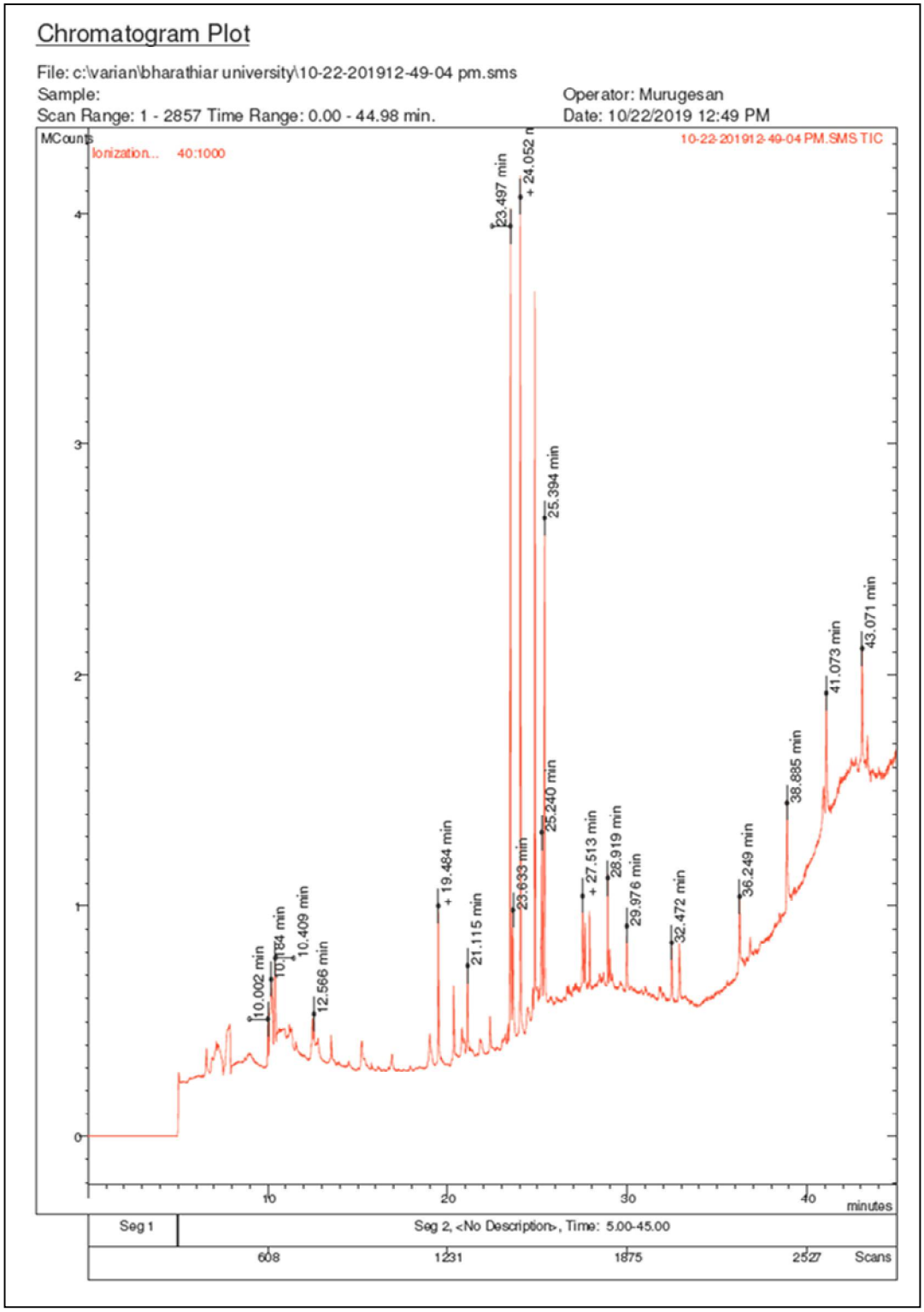


**Figure 1 Showing *C. reflexa* leaf methanolic extractsresult observed for GC-MS analysis**

Plot 1. 10-22-20192-13-39 pm.sms - 10/22/2019 2:13 PM

| | |
|---|---|
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| Slope Sensitivity (SN): | 20 |
| Tangent %: | 10 |
| Peak Size Reject (counts): | 2000 |
| Smoothing: | None |
| Spike Threshold Factor: | None |
| Noise: | Peak to Peak |

| | Retention Time | Area | % of Total | Signal/Noise | Scan Description |
|---|---|---|---|---|---|
| 1. | 19.482 | 3.804e+6 | 3.930 | 169 | Merged |
| 2. | 20.336 | 1.202e+6 | 1.242 | 38 | Merged |
| 3. | 21.116 | 1.936e+6 | 2.000 | 58 | Merged |
| 4. | 23.357 | 894070 | 0.924 | 24 | Merged |
| 5. | 23.502 | 1.634e+7 | 16.877 | 455 | Merged |
| 6. | 23.636 | 1.593e+6 | 1.646 | 20 | Merged |
| 7. | 24.057 | 1.239e+7 | 12.802 | 64 | Merged |
| 8. | 24.870 | 1.671e+7 | 17.263 | 88 | Merged |
| 9. | 25.245 | 6.430e+6 | 6.643 | 56 | Merged |
| 10. | 25.400 | 9.663e+6 | 9.983 | 117 | Merged |
| 11. | 27.512 | 1.095e+6 | 1.132 | 10 | Merged |
| 12. | 27.640 | 1.839e+6 | 1.900 | 16 | Merged |
| 13. | 27.906 | 1.165e+6 | 1.204 | 12 | Merged |
| 14. | 28.924 | 3.472e+6 | 3.588 | 49 | Merged |
| 15. | 29.974 | 2.405e+6 | 2.485 | 40 | Merged |
| 16. | 32.902 | 2.483e+6 | 2.565 | 45 | Merged |
| 17. | 36.248 | 2.831e+6 | 2.925 | 46 | Merged |
| 18. | 38.886 | 3.461e+6 | 3.576 | 36 | Merged |
| 19. | 41.069 | 3.484e+6 | 3.600 | 38 | Merged |
| 20. | 43.063 | 3.126e+6 | 3.229 | 26 | Merged |
| 21. | 43.351 | 469359 | 0.485 | 5 | Merged |

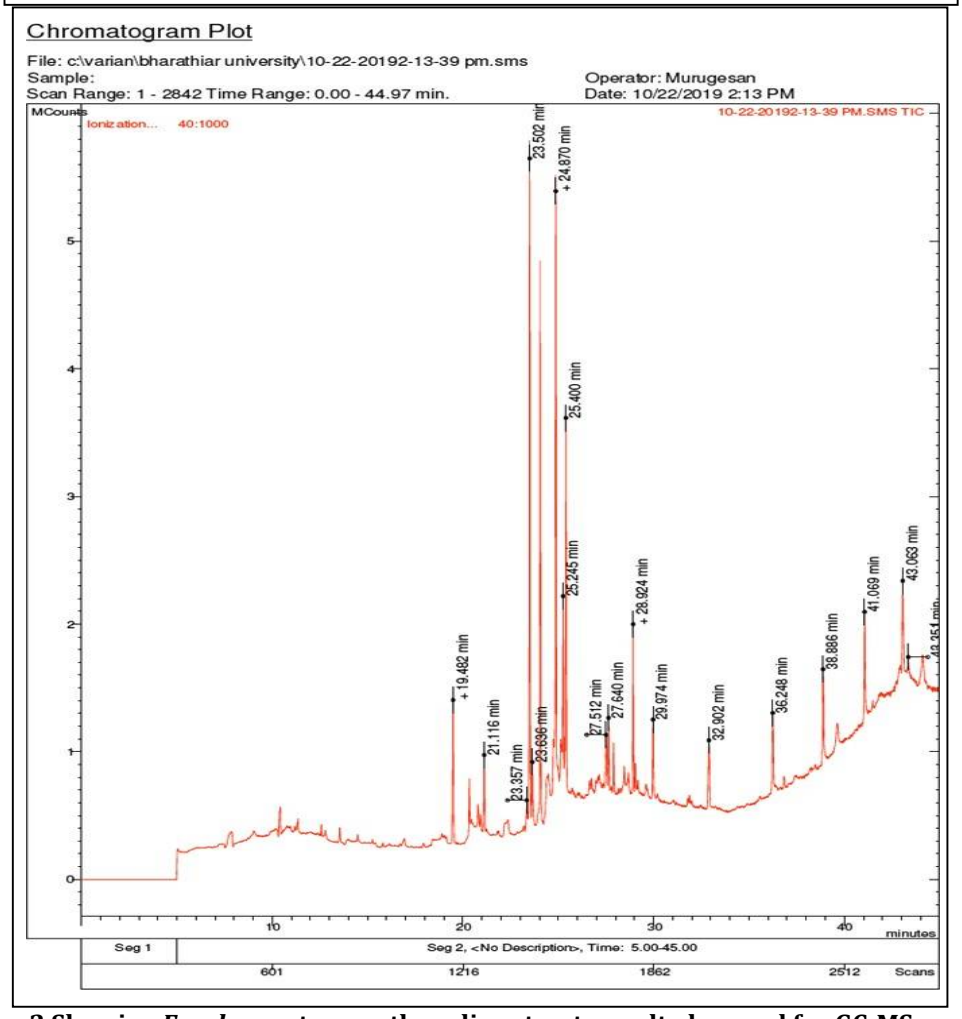


**Figure 2 Showing *F. vulgare* stem methanolic extractsresult observed for GC-MS analysis**

## Plot 1. 10-22-20193-00-15 pm.sms - 10/22/2019 3:00 PM

| | |
|---|---|
| Parameters: | From Data File |
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| Slope Sensitivity (SN): | 20 |
| Tangent %: | 10 |
| Peak Size Reject (counts): | 2000 |
| Smoothing: | None |
| Spike Threshold Factor: | None |
| Noise: | Peak to Peak |

| | Retention Time | Area | % of Total | Signal/Noise | Scan Description |
|---|---|---|---|---|---|
| 1. | 13.542 | 528959 | 0.507 | 27 | Merged |
| 2. | 19.490 | 4.185e+6 | 4.007 | 228 | Merged |
| 3. | 20.350 | 303223 | 0.290 | 15 | Merged |
| 4. | 20.800 | 1.783e+6 | 1.707 | 47 | Merged |
| 5. | 21.118 | 3.424e+6 | 3.279 | 131 | Merged |
| 6. | 23.358 | 570360 | 0.546 | 23 | Merged |
| 7. | 23.506 | 2.082e+7 | 19.933 | 543 | Merged |
| 8. | 23.637 | 3.464e+6 | 3.317 | 47 | Merged |
| 9. | 24.061 | 1.668e+7 | 15.975 | 138 | Merged |
| 10. | 24.740 | 1.122e+6 | 1.074 | 8 | Merged |
| 11. | 24.875 | 2.550e+7 | 24.420 | 259 | Merged |
| 12. | 24.994 | 63788 | 0.061 | 1 | Merged |
| 13. | 25.253 | 1.869e+6 | 1.790 | 19 | Merged |
| 14. | 25.405 | 1.688e+7 | 16.160 | 265 | Merged |
| 15. | 26.970 | 486162 | 0.466 | 6 | Merged |
| 16. | 27.082 | 583026 | 0.558 | 5 | Merged |
| 17. | 27.510 | 2.705e+6 | 2.590 | 14 | Merged |
| 18. | 27.904 | 1.588e+6 | 1.520 | 13 | Merged |
| 19. | 29.052 | 1.229e+6 | 1.177 | 24 | Merged |
| 20. | 41.077 | 652917 | 0.625 | 9 | Merged |

## Chromatogram Plot

File: c:\varian\bharathiar university\10-22-20193-00-15 pm.sms
Sample:
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Operator: Murugesan
Date: 10/22/2019 3:00 PM

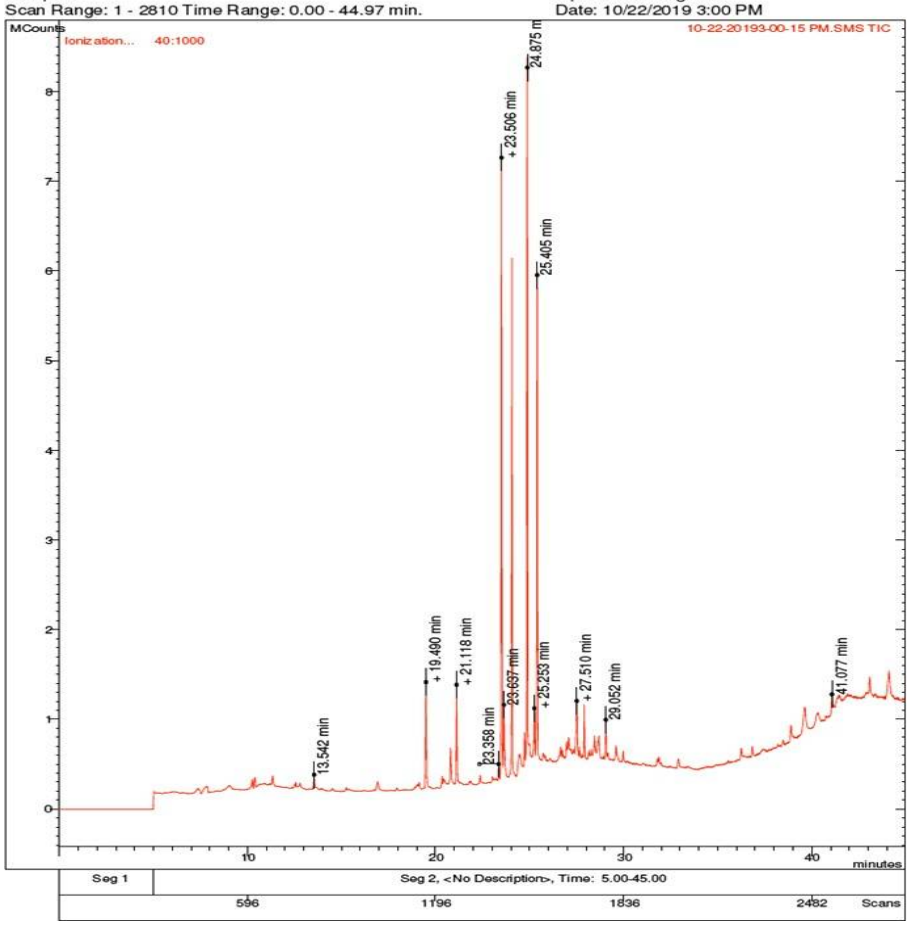


**Figure 3 Showing *T. cordifolia* fruit methanolic extractsresults observed for GC-MS analysis**

## MOLECULAR DOCKING AND SIMULATION STUDIES

Molecular docking studies can be used as a novel inhibitor for treating wastewater treatment. The 3D structure of the CusBA heavy-metal efflux complex and the Phthalic acid is as shown in Figure 4. The docking results for the compounds show strong hydrogen bond associations at the 260 Arg and the 195 Arg positions scoring for 1.88 and 1.91 docking scoresas shown in Figure 5 for its 3D representation and in Figure 6 for its 2D representation. Similarly, Table 2 depicts the interaction results of GC-MS retrieved compounds with heavy metal giving the data on G Score, Dock score and H bond details. The residue details are also given in Table 3, briefly describing the bond length and other major details.

**Table 2 Interaction results of the selected compounds**

| Ligand | G Score | Dock Score | H Bond |
|---|---|---|---|
| Phthalic Acid | -4.2 | -4.2 | -2.82 |
| Ethyl Oleate | -4.44 | -4.44 | 0 |
| Eicasanoic Acid | -3.94 | -3.94 | -1.32 |
| 9-Octadecenoic Acid | -3.64 | -3.64 | -2.35 |
| Hexadecanoic Acid,butyl ester | -3.26 | -3.26 | 0 |
| Eicosaoic Acid | -2.92 | -2.92 | -0.35 |
| Octadecanoic Acid,butyl ester | -2.75 | -2.75 | -0.24 |
| Heptadecanoic Acid | -2.59 | -2.58 | -2.2 |
| Methyl 10-oxohexadecanoate | -2.54 | -2.54 | -0.51 |

**Table 3 Interaction result of top binding affinity ofPhthalic acid with Heavy Metal**

| Protein Name | Ligand Name | InteractingResidue | Bond Length |
|---|---|---|---|
| CusBA heavy-metal efflux Complex | Phthalic Acid | ARG 195, ARG 260 | 1.91,1.88 |

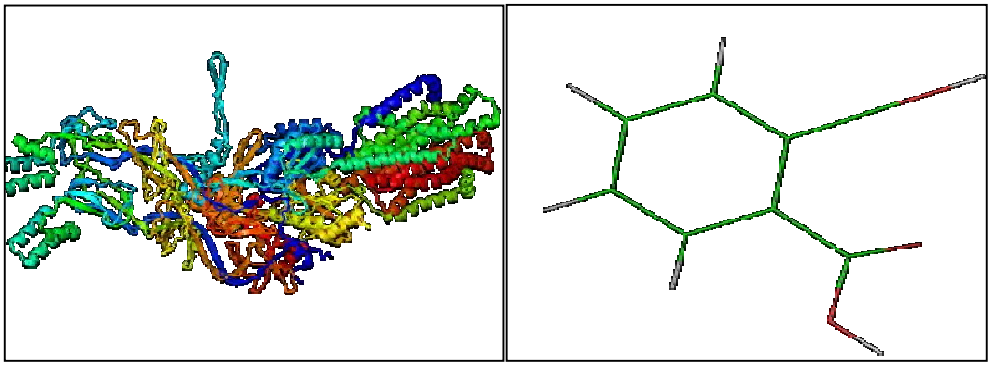

Figure 4 Structure of CusBA heavy-metal efflux complexStructure of Phthalic Acid from ***Escherichia*** *coli*

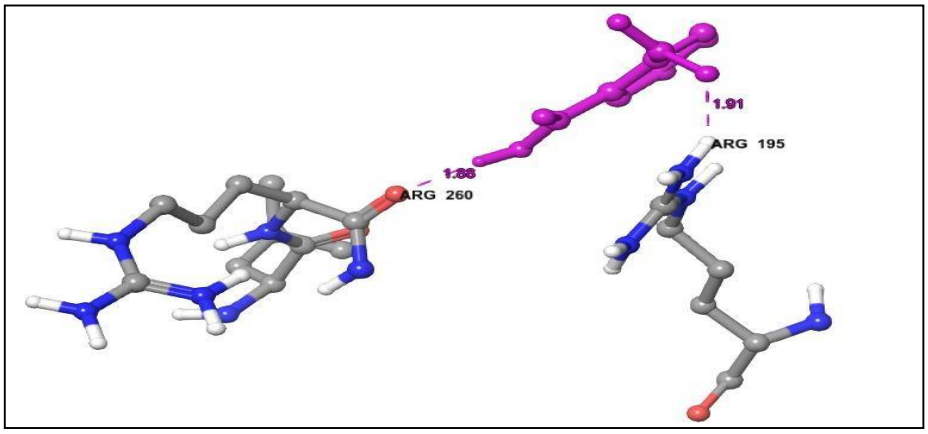


**Figure 5 3D The Docking Structure of CusBA heavy-metal efflux complex from** *Escherichia* ***coli*** **with Phthalic acid. Maroon colour represents ligand (Phthalic acid) molecule and the pink colour dotted line represents hydrogen bond interactionbetween protein and ligand**

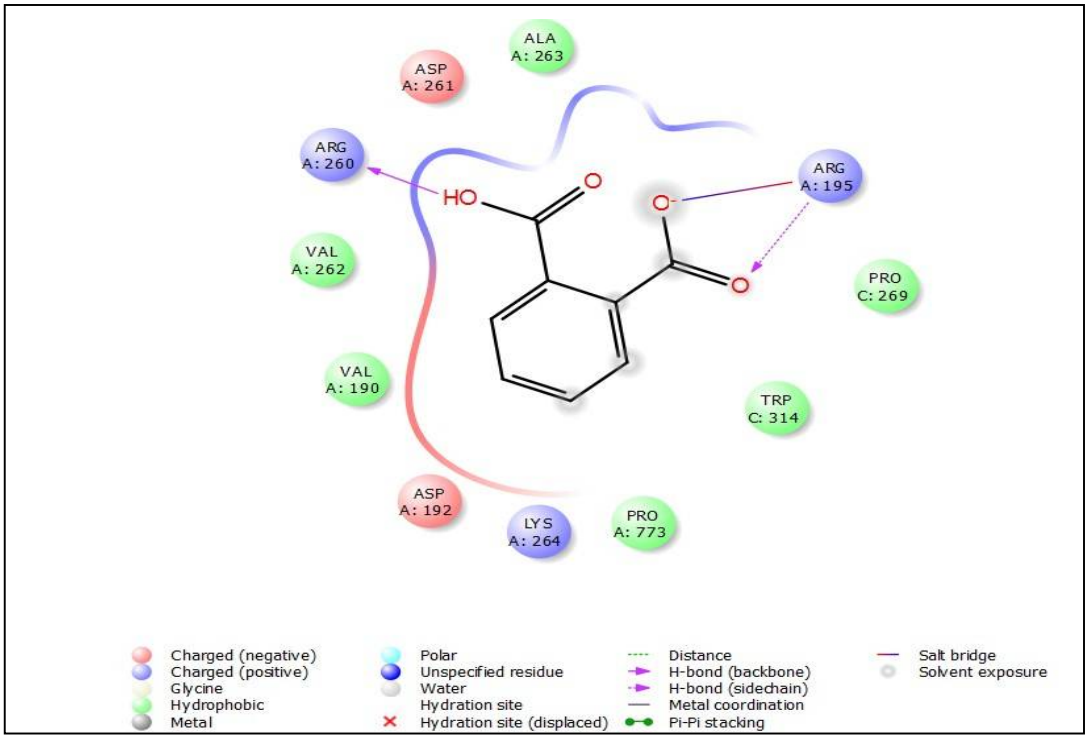


**Figure 6 2D Docking Structure of CusBA heavy-metalefflux complex from *E. coli* with Phthalic acid**

The compound identified in the GC-MS also and it strongly suggests that when the bioactive compounds can be used as naturally remove the pollutant from wastewater and it also for the treatment of wastewater organic wastes.

## CONCLUSION

The GC-MS analysis of methanolic extracts of *C. reflexa* leaves, *F. vulgare* stem and *T. cordifolia* fruits shows the presence of various bioactive components and the molecular docking study was designed order to find the binding efficiency of the derived phytochemical compound from the GC-MS results obtained with the CusBA heavy-metal efflux complex from ***Escherichia*** *coli.* The molecular docking results show that the phthalic acid from the phytochemical derived from the three different plant extracts have been showing better binding activity with the heavy metal complex, which indirectly depicts that the plant extracts have an efficient ability to deteriorate or remove heavy metal toxicants from the solvent effluents and also the phytochemical compound is satisfying Lipinski's rule of 5 and ADMET properties, to be an inhibitor.

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