Table1 : List of Bioactive Compounds in ethanolic extract of Ocimum tenuiflorum (KT)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **R/T (min)** | **Name of the Compound** | **Percentage Abundance** | **Molecular Formula** | **MW (g/mol)** | **3D Structure** |
| 4.4 | Eugenol | 0.31 | C10H12O2 | 164.2 | Eugenol.png |
| 4.69 | Thymol | 13.67 | C10H14O | 150.22 | Thymol.png |
| 5.06 | Caffeic Acid  | 12.83 | C9H8O4 | 180.16 | Caffeic acid.png |
| 7 | Gallic Acid  | 0.61 | C6H2(OH)3COOH | 170.12 | Gallic acid.png |
| 7.5 | Cinnamic Acid | 6.05 | C9H8O2 | 148.16 | Cinnamic acid.png |
| 7.78 | *P*-Coumaric Acid | 7.7 | C9H8O3 | 164.16 | 4-Hydroxycinnamic acid.png |
| 8.94 | Rosmarinic Acid | 2.07 | C18H16O8 | 360.3 | Rosmarinic acid.png |
| 9.33 | Ursolic Acid | 7.4 | C30H48O3 | 456.7 | Ursolic acid.png |
| 9.78 | Oleanolic Acid | 6.09 | C30H48O3 | 456.7 | Oleanolic acid.png |
| 10.43 | Linalool | 20.48 | C10H18O | 154.25 | Linalool.png |
| 10.84 | β-Caryophyllene | 0.17 |  |  | BHW853AU9H.png |
| 11.19 | Carvacrol | 1.49 | C10H14O | 150.22 | Carvacrol.png |
| 11.68 | Catechol  | 11.22 | C6H6O2 | 110.11 | Catechol.png |
| 12.31 | Luteolin | 0.68 | C15H10O6 | 286.24 | Luteolin.png |
| 13.63 | Diosmetin | 0.05 | C16H12O6 | 300.26 | Diosmetin.png |
| 13.93 | Kaempferol | 0.43 | C15H10O6 | 286.24 | Kaempferol.png |
| 15.83 | Apigenin | 0.48 | C15H10O5  | 270.24 | Apigenin.png |
| 18.25 | Rosmarinic Acid | 0.34 | C18H16O8 | 360.3 | Rosmarinic acid.png |
| 18.84 | Genistein | 1.39 | C15H10O5 | 270.24 | Genistein.png |
| 19.4 | Eucalyptol | 0.07 | C10H18O  | 154.25 | Eucalyptol.png |

Table 2: Docking studies between the phytocompounds of KT and biofilm protein of *S. aureus* (3TIP)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **BIOACTIVE COMPOUND** | **PHYTO-CHEMICALS** | **BIOFILM FORMING PROTEIN** | **AUTODOCK RESULTS** | **ENERGY VALUE (∆GO) Kcal/mol** |
| ESSENTIAL OILS | EUGENOL | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip eugenol\AUTODOCK PIC.png | -4.20 |
| THYMOL | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip thymol\AUTODOCK PIC.png | -4.07 |
| TERPENOIDS | OLEANOLIC ACID | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip oleanolic acid\AUTODOCK PIC.png | -6.53 |
| URSOLIC ACID | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip ursolic acid\AUTODOCK PIC.png | -6.42 |
| LINALOOL | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip linalool\AUTODOCK PIC.png | -5.86 |
| β-CARYOPHYLLENE | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip caryophyllene\AUTODOCK PIC.png | -4.40 |
| CARVACROL | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip carvacrol\AUTODOCK PIC.png | -4.09 |
| OTHER PHENOLIC COMPOUNDS | ROSMARINIC ACID | 3TIP *(Staphylococcus aureus)* | E:\docking software\SIR'S WORK\3TIP\3tip rosmarinic acid\AUTODOCK PIC.png | -5.62 |

Table 3: LIGPLOT analysis depicting the major interacting amino acid residues

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **SL. NO.** | **BIOACTIVE COMPOUND** | **PHYTO-CHEMICAL** | **BIOFILM FORMING PROTEIN** | **LIGPLOT** |
| **HYDROPHOBIC BOND** | **HYDROGEN** **BOND** |
| 1. | ESSENTIAL OILS | EUGENOL | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip eugenol\LIGPLOT.PNG | LYS513 (3.95)PRO549 (3.97) | THR516 (2.54)THR516 (3.01) |
| THYMOL | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip thymol\LIGPLOT.PNG | PRO594 (3.41)LEU596 (3.44) | LEU596 (2.74)SER606 (2.90) |
| 2. | TERPENOIDS | OLEANOLIC ACID | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip oleanolic acid\LIGPLOT.PNG | ARG538 (3.23) | LYS525 (2.88) |
| URSOLIC ACID | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip ursolic acid\LIGPLOT.PNG | ARG538 (3.03)VAL541 (3.37) | - |
| LINALOOL | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip linalool\LIGPLOT.PNG | PRO562 (3.40) | GLU564 (2.84)GLU564 (2.84)LYS565 (3.23) |
| Β-CARYOPHYLLENE | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip caryophyllene\LIGPLOT.PNG | PRO549 (3.17)LEU596 (3.50) | - |
| CARVACROL | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip carvacrol\LIGPLOT.PNG | LYS551 (387)PRO594 (3.62)LEU596 (3.87)LEU596 (3.88) | GLY552 (2.72)GLY (2.03)THR (2.46) |
| 3. | OTHER PHENOLIC COMPOUNDS | ROSMARINIC ACID | 3TIP (*Staphylococcus aureus*) | E:\docking software\SIR'S WORK\3TIP\3tip rosmarinic acid\LIGPLOT.PNG | ARG538 (3.75)PRO539 (3.34)VAL541 (3.97) | - |

Table 4: CABS-FLEX analysis showing the major alterations in the interacting residues in presence of phytocompounds

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **SL. NO.** | **BIOACTIVE COMPOUNDS** | **PHYTOCHEMICAL** | **BIOFILM FORMING PROTEIN** | **ROOT MEAN SQUARE FUNCTION** |
| 1. | ESSENTIAL OILS | EUGENOL | 3TIP *(Staphylococcus aureus)* |  |
| THYMOL | 3TIP *(Staphylococcus aureus)* |  |
|  |  |
|  |  |
| 2. | TERPENOIDS | OLEANOLIC ACID | 3TIP *(Staphylococcus aureus)* |  |
|  |  |
|  |  |
| URSOLIC ACID | 3TIP *(Staphylococcus aureus)* |  |
| LINALOOL | 3TIP *(Staphylococcus aureus)* |  |
| β-CARYOPHYLLENE | 3TIP *(Staphylococcus aureus)* |  |
| CARVACROL | 3TIP *(Staphylococcus aureus)* |  |
| 3. | OTHER PHENOLIC COMPOUNDS | ROSMARINIC ACID | 3TIP *(Staphylococcus aureus)* |  |