**Table 1:** MICs of the plant extracts against human pathogens

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Samples | Solvents | | Inhibition zone (mm) | | | | | |
| **Conc.** | ***P. aeruginosa*** | **Conc.** | ***S. aureus*** | **Conc.** | ***S. typhi*** |
| *Pinus roxburghii* | Hexane | | 20 | ND | 0.5 | ND | 1 | ND |
|  | | 25 | 12.33±0.6 | 1 | 12.00 | 10 | 10.33±0.6 |
| Methanol | | 25 | ND | 10 | ND | 1 | ND |
|  | | 30 | 13.67±0.6 | 20 | 11.33±0.6 | 10 | 9.667±0.6 |
| Acetone | | 25 | ND | 10 | ND | 1 | ND |
|  | | 30 | 15.33±0.6 | 20 | 10.67±0.6 | 10 | 12.33±0.6 |
| *Cedrus deodara* | Hexane | | 25 | ND | 0.5 | ND | 1 | ND |
|  | | 30 | 13.33±0.6 | 1 | 9.667±0.6 | 10 | 11.67±0.6 |
| Methanol | | 30 | ND | 1 | ND | 25 | ND |
|  | | 50 | 12.67±0.6 | 10 | 10.33±0.6 | 30 | 11.67±0.6 |
| Acetone | | 30 | ND | 25 | ND | 30 | ND |
|  | | 50 | 10.33±0.6 | 30 | 9.667±0.6 | 50 | 10.67±0.6 |
|  |  | |  |  |  |  |  |  |
| Positive Control |  | | 1 | 19.7±0.6 | 1 | 26.7±0.6 | 1 | 19.7±0.6 |
| Negative Control | |  | 1 | ND | 1 | ND | 1 | ND |

[[1]](#footnote-1)Conc. Concentration (mg/ml)

**Table 2:** Binding affinity of bioactive compounds with bacterial proteases

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Ligand name & ID source | Ligand source | Structural formula | Target protein ID (PDB) | Protein source | Binding affinity |
| Linalool (monoterpenoid)  ZINC1529819 | *P. roxburghii*  (Hexane extract) | ZINC1529819 | 7CO5 | *P. aeruginosa* | -5.5 |
| 4CNN | *S. typhi* | -5.3 |
| 2AS9 | *S. aureus* | -4.9 |
| Ocimene (monoterpenoid)  ZINC1531618 | *C. deodara* (Hexane extract) | ZINC1531618 | 7CO5 | *P. aeruginosa* | -5.7 |
| 4CNN | *S. typhi* | -4.9 |
| 2AS9 | *S. aureus* | -4.8 |
| Bisabolene (sesquiterpenoid)  ZINC13377648 | *P. roxburghii* (Hexane extract) | ZINC13377648 | 2GQC | *P. aeruginosa* | -5.1 |
| 4EZE | *S. typhi* | -7 |
| 2W7S | *S. aureus* | -7.4 |
| Valencene (sesquiterpenoid)  ZINC1734352 | *C. deodara* (Hexane extract) | ZINC1734352 | 2GQC | *P. aeruginosa* | -5.5 |
| 4EZE | *S. typhi* | -6.6 |
| 2W7S | *S. aureus* | -7.7 |
| Limonene  ZINC967513 | *P. roxburghii* (Methanol extract) | ZINC967513 | 7CO5 | *P. aeruginosa* | -6.4 |
| 4CNN | *S. typhi* | -5 |
| 2AS9 | *S. aureus* | -5 |
| Eugenol  ZINC1411 | *C. deodara* (Methanol extract) | ZINC1411 | 7CO5 | *P. aeruginosa* | -5.8 |
| 4CNN | *S. typhi* | -5.3 |
| 2AS9 | *S. aureus* | -5.7 |
| Anethole  ZINC967630 | *P. roxburghii* (Methanol extract) | ZINC967630 | 2GQC | *P. aeruginosa* | -4.5 |
| 4EZE | *S. typhi* | -5.9 |
| 2W7S | *S. aureus* | -5.7 |
| Caryophyllene  ZINC2039864 | *C. deodara* (Methanol extract) | ZINC2039864 | 2GQC | *P. aeruginosa* | -5.7 |
| 4EZE | *S. typhi* | -6.6 |
| 2W7S | *S. aureus* | -7.2 |
| Nortrachelogenin  ZINC900254 | *P. roxburghii* (Acetone extract) | ZINC900254 | 7CO5 | *P. aeruginosa* | -7.2 |
| 4CNN | *S. typhi* | -6.8 |
| 2AS9 | *S. aureus* | -6.7 |
| Taxifolin (flavonoid)  ZINC105076 | *C. deodara* (Acetone extract) | ZINC105076 | 7CO5 | *P. aeruginosa* | -7.6 |
| 4CNN | *S. typhi* | -7.6 |
| 2AS9 | *S. aureus* | -8.3 |

[[2]](#footnote-2)Binding affinity = (kcal/mol)

1. [↑](#footnote-ref-1)
2. [↑](#footnote-ref-2)