**Table S3**: Protein and ligand interactions study of major bioactive compounds obtained from GC-MS study.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **S.No.** | **Compounds Name** | **PubChem ID** | |  | **Binding affinity (Kcal/mol)** |  |
|  |  | |  | **PDF** | **MAPK1** | **SUH** |
| 1. | 2-Methoxy-4-vinylphenol | | 332 | -5.5 | -5.3 | -6.3 |
| 2. | Octanoic acid | | 379 | -5.4 | -4.5 | -4.8 |
| 3. | Indole | | 798 | -5.4 | -5.3 | -5.9 |
| 4. | **Salicylic Acid Methyl Ester** | | **4133** | **-6.2** | **-5.3** | **-6.2** |
| 5. | Hexadecanoic acid, methyl ester | | 8181 | -5.1 | -4.9 | -4.5 |
| 6. | Benzofuran | | 9223 | -5.2 | -5.1 | -5.7 |
| 7. | Hexahydrofarnesyl acetone | | 10408 | -5.6 | -5.3 | -5.5 |
| 8. | Neophytadiene | | 10446 | -5.4 | -5.2 | -5.4 |
| 9. | **Loliolide** | | **100332** | **-5.7** | **-5.9** | **-7.3** |
| 10. | **Eicosapentaenoic acid** | | **446284** | **-6.9** | **-6.3** | **-5.4** |
| 11. | Cyclopentaneundecanoic acid, methyl ester | | 535041 | -5.6 | -5.3 | -5.4 |
| 12. | **Phytol** | | **5280435** | **-6.3** | **-5.5** | **-5.2** |
| 13. | 9,12-Octadecadienoicacid, methyl ester | | 5284421 | -5.7 | -5.1 | -5.4 |
| 14. | Linolenic acid, methyl ester | | 5319706 | -6 | -5.6 | -5 |
| 15. | Z,Z-8,10-Hexadecadien-1-ol | | 5364617 | -5.6 | -5.2 | -4.9 |
| 16. | Methyl stearate | | 8201 | -5.1 | -5.1 | -4.4 |
| 17. | 1-Nonadecene | | 29075 | -4.9 | -4.8 | -4.9 |
| 18. | 2-Methyltetracosane | | 527459 | -5 | -5.2 | -4.9 |
| 19. | Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl) ethyl ester | | 129853056 | -5.3 | -5.5 | -5.1 |