**Table 1:** **List of Antiviral Phytochemicals with Lipinski’s Rules of Drug-Likeness**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| ***S/N*** | ***COMPOUND*** | ***HERBS*** | ***MOLECULAR MASS*** | ***LOG P*** | ***H- BOND DONORS*** | ***H-BOND ACCEPTORS*** | ***MOLAR REFRACTIVITY*** |
|  | Carvacrol | Oregano | 150.00 | 2.82 | 1 | 1 | 46.93 |
| *2* | Safficinolide | Sage | 344.00 | 3.51 | 1 | 5 | 92.08 |
| *3* | Apigenin | Basil (holy) | 270.00 | 2.42 | 3 | 5 | 70.81 |
| *3* | Ursolic | Basil (holy) | 456.00 | 7.09 | 2 | 3 | 132.61 |
| *4* | Trans-Anethole | Fennel | 148.00 | 2.73 | 0 | 1 | 47.70 |
| *5* | Allicin | Garlic | 162.00 | 2.62 | 0 | 1 | 46.00 |
| *6* | Allyl Propyl Disulfide | Garlic | 148.00 | 2.96 | 0 | 0 | 45.40 |
| *7* | Diallyl Trisulfide | Garlic | 178.00 | 3.39 | 0 | 0 | 52.90 |
| *8* | Alanine, 3-(2-Propenylsulfinyl) | Garlic | 177.00 | 0.20 | 3 | 4 | 43.82 |
| *9* | (1s,2r,4s)-(-)-Borneol | Lemon grass | 154.00 | 2.19 | 1 | 1 | 45.24 |
| *10* | Methyleugenol | Lemon grass | 178.00 | 2.43 | 0 | 2 | 53.45 |
| *11* | 3,7-Dimethylocta-1,6-Diene | Lemon grass | 138.00 | 3.55 | 0 | 0 | 48.03 |
| *12* | Neral | Lemon grass | 152.00 | 2.88 | 0 | 1 | 48.49 |
| *13* | Nerol | Lemon grass | 154.00 | 2.67 | 1 | 1 | 49.51 |
| *14* | Menthol | Peppermint | 156.00 | 2.44 | 1 | 1 | 47.35 |
| *15* | Rosmarinic | Peppermint | 360.00 | 1.76 | 5 | 8 | 89.80 |
| *16* | Oleanolic Acid | Rosemary | 456.00 | 7.23 | 2 | 3 | 132.68 |
| *17* | (8Z,13Z)-8,13-Pentadecadien-11-Yn-2-One | *Echinacea* | 218.00 | 4.05 | 0 | 1 | 70.11 |
| *18* | Chlorogenic Acid | *Echinacea* | 354.00 | -0.65 | 6 | 9 | 82.52 |
| *19* | Cynarine | *Echinacea purpurea* | 516.00 | 1.03 | 7 | 12 | 125.20 |
| *20* | Cinnamoyl Echinadiol | *Echinacea purpurea* | 384.00 | 4.53 | 1 | 4 | 110.58 |
| *21* | Sambucus Nigra Degraded Cyanogenic Glycosides (2'-Epimer) | Sambucus nigra | 353.00 | -0.32 | 2 | 9 | 81.67 |
| *22* | Liquiritigenin | Licorice | 256.00 | 2.80 | 2 | 4 | 68.53 |
| *23* | Glabridin | Licorice | 324.00 | 4.00 | 2 | 4 | 91.89 |
| *24* | Zingerone | Ginger | 194.00 | 1.92 | 1 | 3 | 53.66 |
| *25* | Ginsenosides | Ginseng | 444.00 | 7.53 | 2 | 2 | 134.29 |

**Table 2:** **AutoDock Vina score of Antiviral Herbal Compounds on Papain-like Protease with Binding Affinity >8 kcal/mol**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| S/No | African Herb | Active Compound | Country Found |  | Binding Affinity(kcal/mol) | Rmsd/Ub | Rmsd/Lb |
| 1 | Ginseng  (*Pinax ginseng)* | Ginsenosides | Uganda, South Africa |  | -9.9 | 22.018 | 19.332 |
| 2 | Basil Holy *(Ocimum tenuiflorum)* | Ursolic | Nigeria |  | -9.4 | 13.971 | 11.308 |
| 3 | Rosemary*(Salvia Rosmarinus)* | Oleanolic Acid | Nigeria, Sub-Saharan Africa |  | -9.4 | 8.076 | 2.523 |
| 4 | Purple coneflower*(Echinacea purpurea)* | Cynarine | Nigeria Sub-Saharan Africa |  | -8.9 | 5.449 | 3.377 |
| 5 | Licorice*(Glycyrrhiza glabra)* | Glabridin | Nigeria, Ghana, North Africa |  | -8.5 | 6.286 | 4.595 |
| 6 | *Echinacea purpurea*Purple coneflower | Cinnamoyl-Echinadiol | Sub-Saharan Africa |  | -8.2 | 2.134 | 1.512 |

**Table 3. ADMET Analyses of Lead Phytochemicals Using Swiss Tool**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S/N | Compound | Herbs | Formula | Mw | Bioavailability Score | Drug-Like Values  | BBB Permeant | GI - Absorption |
| 1 | Ginsenosides | Ginseng | C30H52O2 | 444.73 | 0.55 | 2 | No | Low |
| 2 | Ursolic | Basil (Holy) | C30H48O3 | 456.7 | 0.56 | 2 | No | Low |
| 3 | Oleanolic Acid | Rosemary | C30H48O3 | 456.7 | 0.56 | 2 | No | Low |
| 4 | Cynarine | *Echinacea Purpurea* | C25H24O12 | 516.45 | 0.11 | 2 | No | Low |
| 5 | Glabridin | Licorice | C20H20O4 | 324.37 | 0.55 | 1 | Yes | High |
| 6 | Cinnamoyl Echinadiol | *Echinacea Purpurea* | C24H32O4 | 384.51 | 0.55 | 2 | Yes | High |
| 7 | Neral | Lemon Grass | C10H16O | 152.23 | 0.55 | 1 | Yes | High |
| 8 | Apigenin | Basil (Holy) | C15H10O5 | 270.24 | 0.55 | 0 | No | High |