**Appendix A. Supplementary data**

**Table S1.** Illustration of the main ImmunoDefender bioactive molecules list, quantities and detailed acceptable daily intake (ADI) compared to 1 ml of bioactive substance in one ampule content product. ADI for each EO ingredient ligands illustrated in milligram per kilogram body weight per day (mg/kg body weight per day).

|  |  |  |  |
| --- | --- | --- | --- |
| **Ingredient** |  **Total substance ingredients (mg)** | **Acceptable daily intake (ADI)****mg/kg body weight per day** | **References** |
| Carvone | 33 | 1.25 | [38] |
| Limonene  | 25.08 | 1.5 | [39] |
| Menthol | 139.41 | 4 | [40] |
| Pipéritone | 64 | No safety concern | [28] |
| α-Phellandrène | 32 | No safety concern | [28] |
| Ocimène | 5.67 | 4 | [42] |
| Pulegone | 13.92 | 0.1 | [43] |
| Menthone | 14 | No safety concern | [28] |
| 1,8 cineole | 102.16 | No safety concern | [28] |
| Eugenol | 49.56 | 1 | [44] |
| Beta caryophyllène | 12.48 | No safety concern | [39] |
| α-humulene | 1 | 0.11 | [45] |
| Eugenyl acetate | 0.72 | No safety concern | [28] |
| Neo-menthol | 8.2 | No safety concern | [28] |
| Menthylacetate | 6.05 | No safety concern | [28] |
| α-terpineol | 27.85 | No safety concern | [28] |
| Α-terpinyl acetate | 9.71 | No safety concern | [28] |
| α-pinene | 1.56 | No safety concern | [28] |
| Cinnamaldéhyde | 46.08 | 1.25 | [35] |
| Cinnamyl acetate | 1.86 | No safety concern | [28] |
| Cinnamtannin B1 | not specified  | not specified  |  |
| Cinnamtannin B2 | not specified  | not specified  |  |
| Pavetanine C1 | not specified  | not specified  |  |
| Tenuifoline  | not specified  | not specified  |  |

**Table S2 :** Free Binding Energy Scores of ImmunoDender Bioactive Compounds Targeting SARS-CoV-2 Main Protease through Molecular Docking Simulations with SwissDock and AutoDock Vina Softwares.

|  |  |  |
| --- | --- | --- |
| **Ingredient** | **Free binding energy score of docking simulated with Mpro via SwissDock (kcal/mol)** | **Free binding energy score of docking simulated with Mpro via AutoDock (kcal/mol)** |
| Carvone | - 4.8 | - 4.5 |
| Limonene  | - 4.7 | - 4.9 |
| Pipéritone | -5 | -4.7 |
| α-Phellandrène | -4.6 | -4.5 |
| Ocimène | - 4.9 | - 4.8 |
| Pulegone | -4.7 | -4.2 |
| Menthone | -5.2 | -4.8 |
| 1,8 cineole | - 4.8 | - 5.1 |
| Eugenol | - 6.8 | - 6.5 |
| Cinnamtannin B1 | -9.5 | - 8.6 |
| Cinnamtannin B2 | -9.4 | - 8.4 |
| Beta caryophyllene | -7 | -6.7 |
| α-humulene | -4.3 | -4.7 |
| Syzyginin B | -10.1 | -9.7 |
| Eugenyl acetate | -6.7 | -6.1 |
| Pavetanine C1 | -10.3 | -9.1 |
| menthol | -6.1 | -5.7 |
| Procyanidin C1 | -9.05 | -8.1 |
| Menthylacetate | - 4.7 | - 4.9 |
| α-terpineol | -5 | -4.6 |
| Comphor | -6.8 | -6.1 |
| α-pinene | -4.7 | -4.9 |
| Cinnamaldéhyde | -7.4 | -6.9 |
| Tenuifoline  | -8.7 | -8.1 |