**Supplementary material**

***Amomum tsao-ko* essential oil, a Novel Anti-COVID-19 Omircon Spike Protein Natural Products: A Computational Study**

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**Table S1** Binding energy of AEO to RBD and NTD.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| AEO | RBDWTa | RBDDeltaa | RBDOmircona |  | NTDWTa | NTDOmircona |
| EO01 | -4.7 | -5.3 | -5.5 |  | -5.4 | -5.9 |
| EO02 | -5.4 | -6.3 | -6.4 |  | -6.7 | -6.8 |
| EO03 | -5.2 | -5.9 | -6.1 |  | -6.1 | -7.1 |
| EO04 | -5 | -5.2 | -5.6 |  | -5.5 | -6 |
| EO05 | -5.2 | -5.4 | -5.5 |  | -5.7 | -5.9 |
| EO06 | -5.3 | -5.9 | -6.3 |  | -6.2 | -6.4 |
| EO07 | -5.2 | -5.3 | -5.5 |  | -5.9 | -6.1 |
| EO08 | -5.7 | -6.5 | -7.0 |  | -7.3 | -7.5 |
| EO09 | -5.4 | -6.4 | -6.2 |  | -6.1 | -7.1 |
| EO10 | -5.6 | -6.4 | -6.5 |  | -6.6 | -7.1 |
| EO11 | -4.1 | -4.5 | -4.5 |  | -4.9 | -5.4 |
| EO12 | -5.2 | -5.4 | -5.6 |  | -5.9 | -6.2 |
| EO13 | -5.7 | -6.1 | -6.1 |  | -5.7 | -6.5 |
| EO14 | -5.5 | -5.7 | -5.7 |  | -6.7 | -7.5 |
| EO15 | -5 | -6.4 | -6.7 |  | -7.4 | -7.8 |
| EO16 | -5.9 | -6.5 | -6.6 |  | -7.2 | -7.5 |
| EO17 | -5.4 | -5.5 | -5.5 |  | -6.2 | -6.6 |
| EO18 | -4.4 | -4.5 | -4.7 |  | -5.3 | -5.8 |
| EO19 | -4.9 | -5.7 | -6.1 |  | -5.8 | -6.6 |
| EO20 | -5.5 | -6.1 | -6.8 |  | -7.4 | -7.1 |

a The unit of binding energy was kJ/mol.

**Fig. S1** Mutation sites of RBDOmicron.



**Fig. S2** Surface representation of the interface formed by the RBD with ACE2.



**Fig. S3** RMSD values of RBD on wild-type (WT) and Omicron mutant.

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**Fig. S4** Molecular interactions of *A. tsao-ko* EO02 against RBDOmicron.



**Fig. S5** Molecular interactions of *A. tsao-ko* EO03 against RBDOmicron.



**Fig. S6** Molecular interactions of *A. tsao-ko* EO07 against RBDOmicron.



**Fig. S7** Molecular interactions of *A. tsao-ko* EO06 against RBDOmicron.



**Fig. S8** Molecular interactions of *A. tsao-ko* EO08 against RBDOmicron.



**Fig. S9** Molecular interactions of *A. tsao-ko* EO09 against RBDOmicron.



**Fig. S10** Molecular interactions of *A. tsao-ko* EO10 against RBDOmicron.

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**Fig. S11** Molecular interactions of *A. tsao-ko* EO16 against RBDOmicron.

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**Fig. S12** Molecular interactions of *A. tsao-ko* EO17 against RBDOmicron.

