**Supplementary materials**

**Computational and In Vitro Evaluation of Sumac-Derived ©Rutan Compounds Towards Sars-CoV-2 Mpro Inhibition**

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**Table S1.** The MMGBSA-based energy estimation for five different Rutan compounds interacting with Mpro

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Replicates** | **R5** | **R6** | **R7** | **R7`** | **R8** |
| 1 |  -94.633  | -56.719  | -65.342 | -98.579  | -103.415  |
| 2 | -103.462  | -109.780  | -45.238  | -84.530  | -104.466  |
| 3 | -76.077  | -110.830  | -70.758  | -96.570  | -119.165  |
| 4 | -79.298  | -83.335  | -83.948  | -95.421  | -90.664  |
| 5 | -52.105  | -108.105  | -70.931  | -85.466  | -104.103  |
| **Average** | **-81.115**  | **-93.754**  | **-67.243**  | **-92.113**  | **-104.363**  |