**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

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| --- | --- | --- | --- | --- | --- |
| **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** |