**Table S2.**  Structure-activity relationship (SAR) of the most potent compounds.

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound Name** | ***In silico* anti-tyrosinase effect** | ***In vitro* anti-tyrosinase effect** | **References** |
| Vanillic acid | Ki values of 428.75 nM | IC50 values of 15.84 mM | Girawale, et al. 2022 |
| Deoxyarbutin | Ki values of 37.61 µM | IC50 values of 57.70 µM | Chawla et al. 2008 |
| Kojic acid | Ki values of 573.31 µM | IC50 values of 40.69 µM | Chen et al. 2015 |