

Chompoonuch Tancharoen 2012: Experimental and Theoretical Studies on Resveratrol Oligomer Compounds from the Bark of Dipterocarpaceae Family against HIV-1 Reverse Transcriptase. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Songwut Suramitr, Ph.D. 82 pages.

In this work, a new resveratrol trimer together with three known compounds were isolated including Gnetin C, Anigopreissin A and Hopeafuran from the stem-bark of *Shorea siamensis* Miq. All isolated compounds were evaluated for their anti-HIV-1 reverse transcriptase by using Nevirapine as reference drug. From the IC_{50} values, it showed that Anigopreissin A can inhibit wild-type HIV-1 RT activity as same as Nevirapine. In addition, orientations of all isolated compounds were investigated by molecular docking simulations. The results of GoldScore were found in the order of a new resveratrol trimer (83.40) > Anigopreissin A (65.39) > Gnetin C (60.63) > Nevirapine (62.82) > Hopeafuran (19.81). IC_{50} results of a new resveratrol trimer corresponded to partial interaction. Whereas, the results of partial interaction and docking calculations of the other ligands contravened to the experimental IC_{50} values. Thus, a new resveratrol trimer and Anigopreissin A are found to be potent compounds to further study as novelistic drugs.

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