Polygonumins A, a newly isolated compound from the stem of Polygonum minus Huds with potential medicinal activities

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Abstract
Polygonumins A, a new compound, was isolated from the stem of Polygonum minus. Based on NMR results, the compound's structure is identical to that of vanicoside A, comprising four phenylpropenoid ester units and a sucrose unit. The structure differences were located at C-3.""": The cytotoxic activity of polygonumins A was evaluated on several cancer cell lines by a cell viability assay using tetrazolium dye 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT). The compound showed the highest antiproliferative (p < 0.05) activity against K562 (Human Leukaemia Cell Line), MCF7 (Human breast adenocarcinoma cell line), and HCT116 (Colorectal cancer cells). Cytotoxic studies against V73-4 cells were carried out and showed that polygonumins A was toxic at 50 μg/mL, suggesting that this compound may be used as an anticancer drug without affecting normal cells. Polygonumins A also showed promising activity as an HIV-1 protease inhibitor with 56% relative inhibition. Molecular docking results indicated that the compound possesses high binding affinity towards the HIV protease over the low binding free energy range of -10.5 to -11.3 kcal/mol. P. minus is used in Malaysian traditional medicine for the treatment of tumour cells. This is the first report on the use of P. minus as an HIV-1 protease inhibitor.

Keywords
KeyWords Plus: ESSENTIAL OIL; VANICOSIDE-B; ACETYLCHOLINESTERASE ACTIVITY; PHENYLPROPENOID GLYCOSIDES; INHIBITORY ACTIVITIES; BIOLOGICAL ACTIVITIES; IN-VITRO; ANTI-HIV; ANTI-INFLAMMATORY; ANTI-HIV-1

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