Supplementary Materials

Placovinane: 1″β-Ethoxy-6,4′-dimethoxy-3″,3″-dimethyl-1″,2″-dihydropyranoisoflavone, a New Isoflavone Derivative

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Abstract: Isoflavonoids possess a 3-phenylchroman skeleton and are the biologically active secondary metabolites of various plants that are being used for various health promoting and restoring effects through various mechanisms. Chromatographic separation of the n-hexane extract from the stems of Placolobium vietnamense led to the isolation of a new isoflavone derivative, placovinane (1), together with four known compounds (2-5). The structures of isolated compounds were identified from their spectroscopic data and by comparison with the literature. All isolated compounds were evaluated for their α-glucosidase inhibition. They all exhibited potent α-glucosidase inhibition with IC_{50} values ranging from 11.0 to 87.3 μM, which was significantly less than the positive control acarbose (IC_{50} 179 μM). The cytotoxicity of 1 was evaluated against KB, Hep G2, and MCF7 cell lines, and displayed weak cytotoxicity toward KB and Hep G2 cell lines, with the IC_{50} values of 89.6 and 93.8 μM, respectively.

Keywords: Placolobium vietnamense, placovinane, isoflavone derivative, α-glucosidase inhibition, cytotoxicity
Figure S1. The $^1$H NMR spectrum of 1 in DMSO-$d_6$.
Figure S2. The $^{13}$C NMR spectrum of 1 in DMSO-$d_6$

Figure S3. The COSY spectrum of 1
Figure S4. The HSQC spectrum of 1
Figure S5. The HMBC spectrum of 1
**ANALYSIS REPORT**

**Injection details**

- **Sample name**: LIEN206
- **Vial position**: 18
- **Sample file name**: SER. wh22 – LIEN
- **Inject volume**: 5.00 µL
- **Acquisition date**: 01/09/2020 10:33:36 AM
- **Acquisition method**: ESI_POS_SCAN
- **Operator**: CB21261708
- **Instrument name**: X500q QTof

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**Full mass spectrum**

Spectrum from LIEN206 (sample 1) - LIEN206 (1+1ESI, +TOF MS (50 - 1500)) from 0.162 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

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**Expanded spectrum**

Spectrum from LIEN206 (1+1ESI wh22 (sample 1) - LIEN206 (1+1ESI, +TOF MS (50 - 1500)) from 0.162 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

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**Figure S6.** The HRESIMS spectrum of 1