SUPPLEMENTARY MATERIAL

Cytotoxic Activity and Molecular Docking of a Novel Biflavonoid Isolated from *Jacaranda acutifolia* (Bignoniaceae)

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Abstract

A novel biflavonoid [kaempferol (6→8") apigenin] was isolated from the leaves of *Jacaranda acutifolia*. The structure was elucidated based on chemical evidence, 1D and 2D spectroscopic analyses as well as spectrometric techniques. The compound showed promising cytotoxic activity against breast cancer cell line MCF-7. The anticancer activity was explained via virtual docking of the isolated compound to the main sites in the human cyclin-dependent kinase2 (CDK2) crystal structure.

Keywords: *Jacaranda acutifolia*, Bignoniaceae, biflavonoid, cytotoxic activity, molecular docking.

UV spectrum (MeOH) and NaOMe shifting reagent of compound **1** Kaempferol (6→8'') apigenin.

^1H -NMR of compound **1**: Kaempferol (6 $\rightarrow$ 8'') apigenin, $\text{DMSO}-d_6$.

¹H-NMR of compound **1**: Kaempferol (6→8'') apigenin, DMSO-*d*₆ + D₂O.

JBL-18_APT2_500
STANDARD CARBON PARAMETERS

APT spectrum of compound **1**: Kaempferol (6→8'') apigenin.

COSY of compound 1: Kaempferol (6→8'') apigenin.

HMBC of compound 1: Kaempferol (6→8'') apigenin.

HMBC of the aromatic region of compound **1**: Kaempferol (6→8'') apigenin.

HSQC of compound 1: Kaempferol (6→8'') apigenin.

HSQC of the aromatic region of compound **1**: Kaempferol (6→8'') apigenin.

(+)-ESI-MS of compound **1**: Kaempferol (6→8'') apigenin