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.
$^1$H-NMR of compound 1: Kaempferol (6→8") apigenin, DMSO-$d_6$. 
$^1$H-NMR of compound 1: Kaempferol (6→8") apigenin, DMSO-$d_6$ + D$_2$O.
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
