SUPPLEMENTARY MATERIAL

New jacaranone glucoside from *Jacaranda oxyphylla* leaves

V.V. Pereira<sup>ab</sup>, L.P. Duarte<sup>a</sup>, R.R. Silva<sup>c</sup>, J.A. Takahashi<sup>a</sup>

<sup>a</sup>Chemistry Department, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, Brazil; <sup>b</sup>Faculty of Pharmacy, Universidade Federal de Minas Gerais, 31270-901, Belo Horizonte, Brazil; <sup>c</sup>Chemistry Department, Universidade Federal dos Vales do Jequitinhonha e Mucuri, 39100-000, Diamantina, Brazil

* Corresponding author. E-mail: vncsviana@yahoo.com.br

* *Jacaranda oxyphylla* Cham. is popularly known as “caroba-de-São-Paulo” and it is used in traditional medicine for microbial infections. A new phytoquinoid (α/β-glucoside-4-phenylacetate-6-(1-hydroxy-4-oxo-2,5-cyclohexadiene-1-acetate) (1) was isolated from *J. oxyphylla* leaves, together with three known compounds: quercetin-3-O-β-D-galactoside (2), verbascoside (3) and polystyrene (4). Their chemical structures were elucidated using spectroscopic techniques and by comparison with the related known compounds. In addition, it was found a pronounced acetylcholinesterase inhibitory activity for the quinoid 1 (100.0 ± 0.8%) and phenolic compounds 2 and 3 (99.9 ± 0.7% and 99.3 ± 0.5%, respectively), if compared to the standard eserine (92.7 ± 0.4%), that was analyzed by a microplate spectrophotometer.

**Keywords:** Bignoniaceae, *Jacaranda oxyphylla*, quinoid, antiacetylcholinesterase activity.
**Figure S1** – The HR-ESIMS(+) spectrum of compound 1.

**Figure S2** – IR spectrum (KBr 1%) of compound 1.
Figure S3 – $^1$H NMR spectrum (400 MHz, acetone-$d_6$) of compound 1.

Figure S4 – $^{13}$C NMR spectrum (100 MHz, acetone-$d_6$) of compound 1.
Figure S5 – DEPT spectrum (100 MHz, acetone-$d_6$) of compound 1.

Figure S6 – HSQC (400 MHz, acetone-$d_6$) of compound 1.
Figure S7 – HMBC (400 MHz, acetone-d$_6$) of compound 1.
Figure S8 – Key HMBC correlations (→) for the compound 1.
Table S1 – NMR spectral data for compound 1 in acetone-$d_6$ with assignments supported by DEPT, COSY, HSQC and HMBC ($\delta$ in ppm, J in Hz).

| Position | Multip. | $\delta^1_C$ | $\delta^1_H$ | HMBC |
|----------|---------|--------------|--------------|------|
| 1$\alpha$ | CH      | 97.2         | 4.55 (d, J = 3.6) | -    |
| 1$\beta$ | CH      | 92.6         | 5.15 (d, J = 7.6) | -    |
| 2        | CH      | 72.8         | 3.46 (m)      | H-1  |
| 3        | CH      | 74.3         | 3.63 (m)      | H-4  |
| 4        | CH      | 71.4         | 4.84 (m)      | H-5  |
| 5        | CH      | 71.6         | 3.87 (m)      | H-4,H-6 |
| 6        | CH$_2$ | 63.0         | 4.03 (m)      | H-4  |
| 1$'$     | C       | 134.6$^*$    | -             | H-7', H-2', H-3', H-5', H-6' |
| 2$'$     | CH      | 129.4        | 7.30 (m)      | H-3', H-5', H-6', H-7' |
| 3$'$     | CH      | 128.3        | 7.30 (m)      | H-2', H-5', H-6' |
| 4$'$     | CH      | 128.8        | 7.25 (m)      | H-2', H-3', H-5', H-6' |
| 5$'$     | CH      | 128.3        | 7.30 (m)      | H-2', H-3', H-6' |
| 6$'$     | CH      | 129.4        | 7.30 (m)      | H-3', H-5', H-6', H-7' |
| 7$'$     | CH$_2$ | 40.6         | 3.65 (m)      | H-2', H-3', H-5', H-6' |
| 8$'$     | C       | 170.5        | -             | H-4,H-7' |
| 1$''$    | C       | 66.9         | -             | H-3'', H-5'', H-7'' |
| 2$''$    | CH      | 150.4        | 7.06 (m)      | H-6'', H-7'' |
| 3$''$    | CH      | 127.2        | 6.08 (m)      | H-5'' |
| 4$''$    | C       | 184.8        | -             | H-2'', H-6'' |
| 5$''$    | CH      | 127.2        | 6.08 (m)      | H-3'' |
| 6$''$    | CH      | 150.5        | 7.06 (m)      | H-2'', H-7'' |
| 7$''$    | CH$_2$ | 44.7         | 2.76 (m)      | -    |
| 8$''$    | C       | 168.3        | -             | H-6, H-7'' |

Multip. = Multiplicity; $^*$100 MHz for $^{13}$C NMR; $^5$400 MHz for $^1$H NMR; $^6$signal based on HMBC.