

**Table S3.**  $^{13}\text{C}$  and  $^1\text{H}$  NMR nuclear magnetic resonance assignments of 3-Oxo-voacangine (TcK005) isolated from the ethanol extract of seeds of *Tabernaemontana cymosa* Jacq., comparing to those reported in the literature.

| Carbon                          | TcK005          |              | [1]             |              | [2]             |              |
|---------------------------------|-----------------|--------------|-----------------|--------------|-----------------|--------------|
|                                 | $^{13}\text{C}$ | $^1\text{H}$ | $^{13}\text{C}$ | $^1\text{H}$ | $^{13}\text{C}$ | $^1\text{H}$ |
| 2                               | 134,65          |              | 134,5           |              | 136             |              |
| 3                               | 173,07          |              | 172,8           |              | 176             |              |
| 5                               | 42,72           |              | 42,6            |              | 42,7            |              |
| 6                               | 21,18           |              | 21              |              | 21,2            |              |
| 7                               | 109,22          |              | 108,8           |              | 109,5           |              |
| 8                               | 128,23          |              | 127,9           |              | -               |              |
| 9                               | 100,48          | 6,95         | 100,2           | 6,9          | 100,1           | 6,93         |
| 10                              | 154,21          |              | 153,8           |              | 154,0           |              |
| 11                              | 112,59          | 6,84         | 112,3           | 6,81         | 112,7           | 6,83         |
| 12                              | 111,38          | 7,16         | 111,2           | 7,37         | 111,6           | 7,16         |
| 13                              | 130,83          |              | 130,7           |              | 130             |              |
| 14                              | 35,97           |              | 35,2            |              | 38,4            |              |
| 15                              | 31,03           |              | 30,8            |              | 31              |              |
| 16                              | 56,11           |              | 55,4            |              | 56,7            |              |
| 17                              | 35,49           |              | 35,7            |              | 36              |              |
| 18                              | 11,41           | 0,97         | 11,8            | 0,86         | 11,1            | 1            |
| 19                              | 27,67           |              | 27,5            |              | 27,6            |              |
| 20                              | 38,21           |              | 38              |              | 35,6            |              |
| 21                              | 56,02           |              | 55,8            |              | 56,1            |              |
| 22                              | 175,60          |              | 175,6           |              | 172,9           |              |
| CO <sub>2</sub> CH <sub>3</sub> | 53,09           | 3,77         | 52,8            | 3,7          | 53              | 3,75         |
| OCH <sub>3</sub>                | 55,60           | 3,88         | 55,9            | 3,81         | 56,1            | 3,88         |

1. Sharma, P.; Cordell, G.A. Heyneanine hydroxyindolenine, a new indole alkaloid from *Ervatamia coronaria* var. plena. *Journal of natural products* **1988**, *51*, 528-531.
2. Goncalves, M.d.S.; Braz-Filho, R.; Mathias, L.; Vieira, I.J.C. Chemical constituents of *Tabernaemontana catharinensis* (apocynaceae).