

Poster

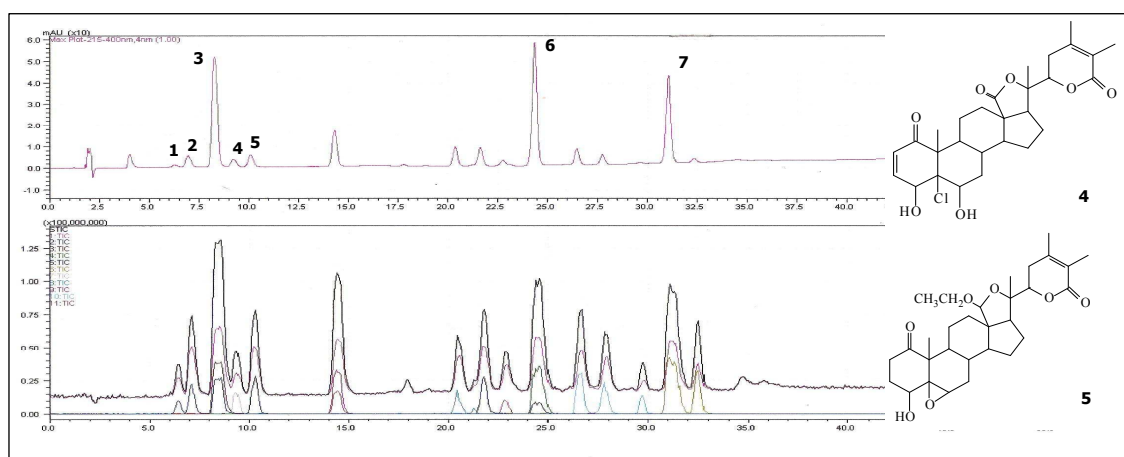
## Characterization of bioactive withaphysalins from leaves of *Acnistus arborescens* by LC-HRMS-IT-TOF

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Plants of the genus *Acnistus* (Solanaceae) biosynthesize a complex group of biologically active C<sub>28</sub> steroidal lactones denominated withasteroids. As part of a collaborative search program to identify novel naturally occurring anticancer agents from plant, the investigation of *Acnistus arborescens* was undertaken.<sup>1,2</sup> This plant, in folk medicine, exhibits different therapeutic uses, for instance, the infusion of its leaves is used to treat bruises, contusions and sprains. The treatment of liver and spleen diseases and cancerous growths are also reported.<sup>3</sup> Previous studies have led to the isolation of several cytotoxic withanolides,<sup>3</sup> including new withaphysalins, to which the cytotoxic effects against several tumor cell lines have been reported.<sup>1,2</sup> To obtain qualitative information about the chemical composition of a cytotoxic fraction rich in withaphysalins, 0.2 µg/L of this fraction, obtained from leaves of *A. arborescens*, was analyzed by the positive ion mode LCMS/MS-IT-TOF (Shimadzu ion trap time-of-flight hybrid mass spectrometer) with a flow rate 1.5 mL/min and 30% MS<sup>n</sup> CID energy (Figure 1). Seven withaphysalins were identified (**1-7**), two of which have not been previously isolated (**4** and **5**). The other five previously isolated, have been characterized by NMR (1D and 2D) data. The structures of both unknown withaphysalins were characterized based on their high resolution tandem mass spectra and by comparison of the data to the characteristic fragmentation pattern of the analogous withaphysalins. Therefore, this method provided a fingerprint of the withaphysalins of this important cytotoxic species.



**Figure 1:** LC-MS chromatogram of a fraction from *A. arborescens* rich in withaphysalins.

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[2] Veras, M. L.; Bezerra, M. Z. B.; Braz-Filho, R.; Pessoa, O. D. L.; Montenegro, R. C.; Pessoa, O. C.; Moraes, M. O.; Costa-Lotufo, L. V.; *Planta Med.* **2004**, *70*, 551.

[3] Minguzzi, S.; Barata, L. E. S.; Shin, Y. G.; Jonas, P. F.; Chai, H. B.; Park, E. J.; Pezzuto, J. M.; Cordell, G. A.; *Phytochemistry* **2002**, *59*, 635.