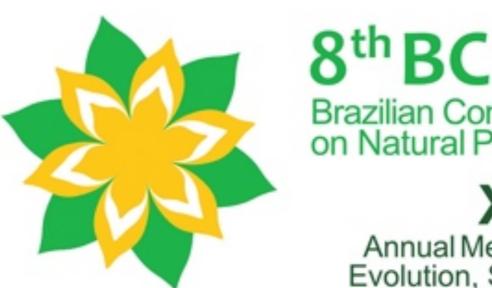
Cytotoxic anthraquinones from a Brazilian cave soil-derived fungus *Aspergillus* sp. SDC28



Annual Meeting on Micromolecular Evolution, Systematics and Ecology



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INTRODUCTION

Caves are subterranean environments considered extreme environments with permanent darkness, high humidity, constant temperature, providing highly specialized niches. Moreover, this kind of environment has been overlooked regarding its potential for new genetic resources. 1-4 Isolation and screening of new fungal strains from extreme environments, such as caves, is a promising approach to find new bioactive metabolites. The investigation of the extract of the growth medium EtOAc produced by the soil-derived fungus *Aspergillus* sp. SDC28, isolated from a Brazilian cave, yielded two anthraquinones, versicolorin C (1) and versiconol (2). The complete assignment of NMR and mass spectroscopic data has been performed. The absolute configuration of both compounds was unambiguously established by the analysis of experimental and theoretical electronic circular dichroism (ECD) data. Compounds 1 and 2 were found to exhibit cytotoxic activity against human ovarian cancer cells (OVCAR3).

EXPERIMENTAL SECTION

The soil-derived fungus *Aspergillus* sp. SDC28 was isolated from Catão cave (São Desidério karst area, state of Bahia - Brazil). Compounds were isolated as shown in Figure **1**.

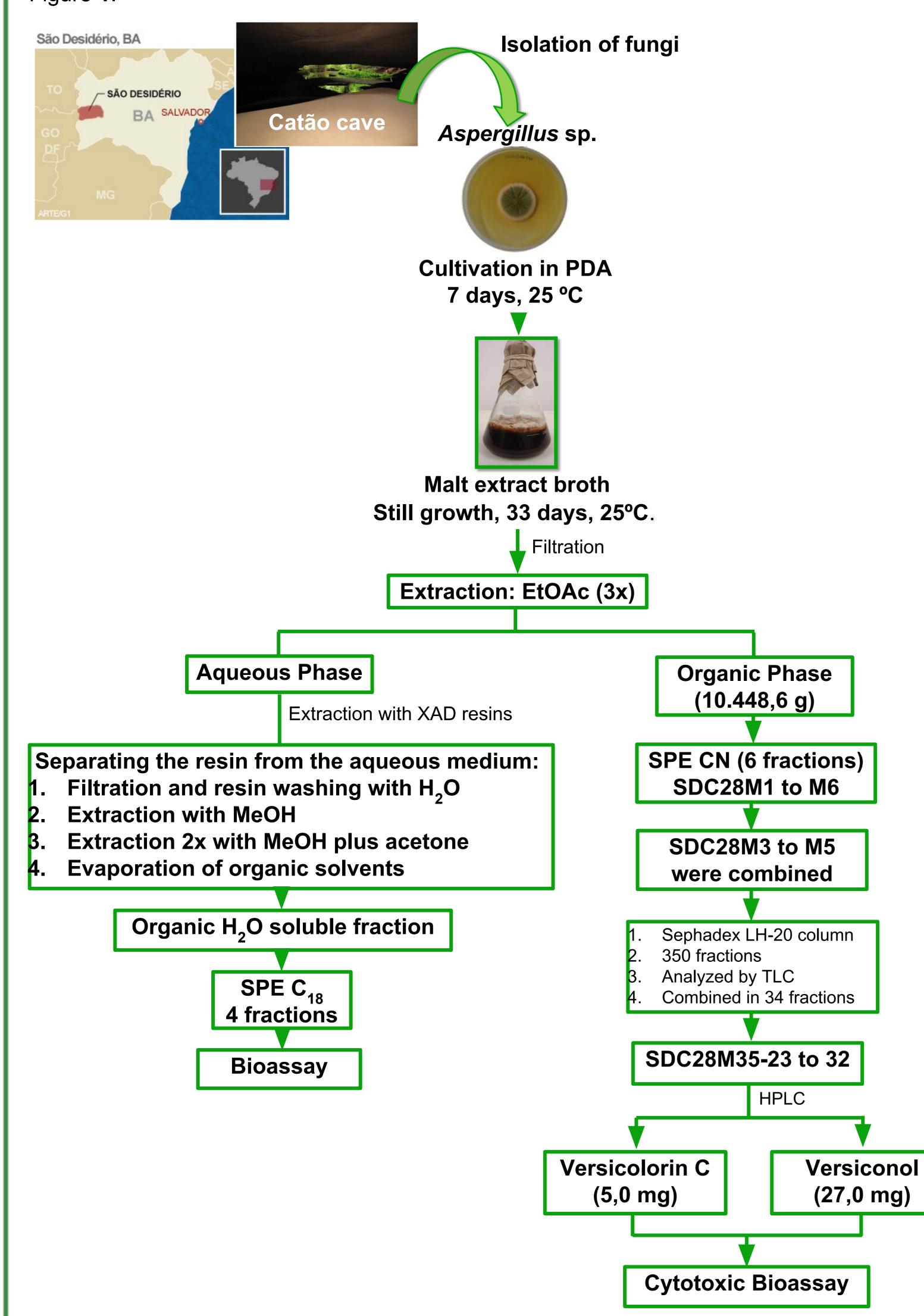


Figure 1. Method for isolation of versicolorin C and versiconol.

RESULTS and DISCUSSION

Compounds 1 and 2 have been previously isolated from cultures of *A. versicolor*, *A. parasiticus*, *Aspergillus* sp. F40, *A. ustus* and *A. nidulans*. However, it is the first time the absolute configuration of 1 and 2 has been established and have been tested for in vitro antiproliferative activity against human ovarian cancer cells OVCAR3.

The excellent agreement between observed and simulated UV/ECD data allowed the unambiguous assignment of compound (+)-1 as 1'R,2'S and (+)-2 as 2'S.

CONCLUSION

In summary, we report for the first time the absolute configuration of versicolorin C (1) and versiconol (2) isolated from cultures of *Aspergillus* sp. SDC28. Both compounds 1 and 2 displayed significant cytotoxic activity against human ovarian cancer cells OVCAR3.

ACKNOWLEDGMENTS

NOEDiff ¹H ¹H







Conf 4. +0.21 kcal/mol (21%)

REFERENCES

¹Paula, C. C. P. et al. (2019). *An. Acad. Bras. Cienc.*, **91**.

²Paula, C. C. P. et al. (2016). *J. Cave Karst Stud.*, **78** (3), 208-217.

³Northup, D. E.; Lavoie, K. H. (2001). *Geomicrobiol. J.*, **18**, 199-22.

⁴Taylor, E. L. S; Stoianoff, M. A. A. R.; Ferreira, R. L. (2013). *Int. J. Speleol.*, **42** (3), 267-277.