UiT
THE ARCTIC UNIVERSITY OF NORWAY

A Novel Brominated Alkaloid Securidine A isolated from the marine bryozoan *Securiflustra securifrons*

Priyanka Michael [1], Kine Ø. Hansen [1], Johan Isaksson [2], Jeanette H. Andersen [1] and Espen Hansen[1]
[1]MARBIO, UiT – The Arctic University of Norway, Brevika, N-9037, Tromsø, Norway
[2]Department of Chemistry, UiT – The Arctic University of Norway, Brevika, N-9037, Tromsø, Norway

STUDY BACKGROUND

Marine bryozoans are producing a significant number of bioactive secondary metabolites including macrolides, alkaloids, sterols and heteroatom-containing compounds that possess antitumor, antibacterial and muscle relaxant activities [1,2].

In the present study, we isolated and elucidated the structure of the brominated tyrosine derivative Securidine A from the coldwater marine bryozoan *Securiflustra securifrons,* and its bioactivities were also investigated by selected bioassays. Previously, nine compounds were isolated from *S. securifrons* and no biological activities were reported [3,4].

METHODOLOGY

- *S. securifrons* was collected in the North Sea (71,0759° N, 24,4355° E)
- The frozen marine bryozoan was extracted and pre-fractionated by flash chromatography
- The fractions were assayed for cytotoxicity against A2056 human melanoma and HT29 colon carcinoma cancer cell lines and the active fractions were analyzed using HR-MS
- The elemental composition of Securidine A was calculated using UHPLC-HR-MS and followed by dereplication
- Purification was carried out on two different columns, Waters Xterra RP18 (10×300 mm, 10 µm) and Waters Phenyl-hexyl Prep (10×250 mm, 5 µm) in Prep-HPLC
- The structure of Securidine A was elucidated based on 1D and 2D NMR experiments
- The bioactivity of Securidine A was tested using different bioassays such as cytotoxic, antibacterial, and anti-diabetic activities as well as its potential for biofilm inhibition.

WORK SCHEME

Collection of Marine bryozoan

Extraction

Prefractionation

Screening of bioactivity

High Resolution Mass Spectrometry (HR-MS) analysis

Dereplication (Novel/or Known compound)

Isolation by Prep-HPLC

Structure elucidaion by Nuclear Magnetic Resonance (NMR)

Bioactivity profiles

Anticancer
Antibacterial
Antidiabetes
Inhibtion of Biofilm growth

RESULTS

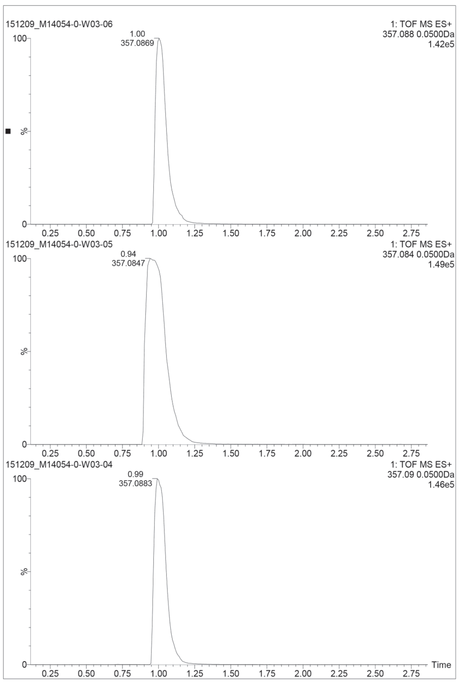

Figure:1 - Ion chromatogram of active flash fractions (4 to 6) of *S.securifrons* showed the target compound with mass 357.0926 *m/z.*

Dereplication: (Figure 1)

The active fractions (4 to 6) were analysed by UHPLC-HR-MS. The isotopic pattern indicated that the eluted compound was a mono-brominated compound and its elemental composition was $C_{14}H_{21}BrN_4O_2$. The target compound was dereplicated based on data base search, which was suggested that the compound was new.

Isolation: (Figure 2)

Preparatrive HPLC was used to isolate Securidine A. The mass of Securidine A (357.0926 *m/z*) was used as a collection trigger. The active fractions of *S.securifrons* were loaded onto a Waters - Xterra RP18 and Phenyl - hexyl Prep HPLC columns.

The purified compound was used for structure elucidation and to investigate its biological activities.

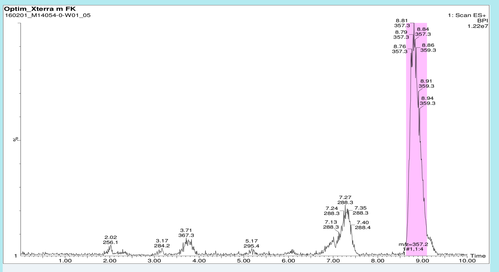

Figure:2 - Base peak intensity chromatogram showed the successful isolation of the target compound.

Structure Elucidation: (Figure 3)

The structure of the isolated compound was determined through interpretation of data from 1D and 2D (HMBC, ME-HSQC, H2BC, COSY and ROESY) NMR experiments. We have named the new compound 'Securidine A'. 2D correlations of Securidine A is seen in the figure below.

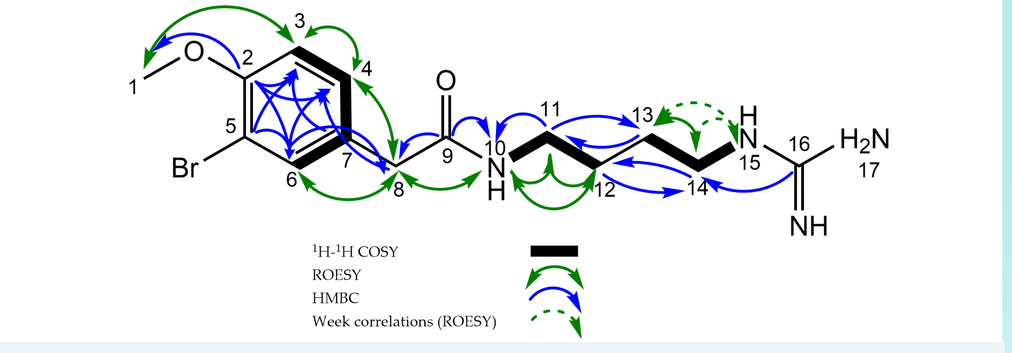

Figure:3 - The Key HMBC, ME-HSQC, H2BC, COSY and ROESY correlations of Securidine A

Summary:

The new brominated tyrosine derivative Securidine A was isolated from the aqueous extract of the marine bryozoan *Securiflustra securifrons*. The structure was determined by interpretation of data from 1D and 2D NMR experiments and mass spectrometry analysis. Securidine A did not show any biological activities in the applied bioassays. Further bioactivity profiling is required in order to identify any potential biological activities of the molecule.

Aknowledgement:

The authors would like to thank Marbank for marine bryozoan collection, identification and extraction preparation.
The study was supported by the Research council of Norway, Grant no. 174885/130.

References:

1). Sinko, J.; Rajchard, J.; Balounova, Z.; Fikotova, L.. Vet. Med. Czech 2012, 57, 177-184.
2). Tadesse, M.; Tabudravu, J.N.; Jaspars, M.; Strom, M.B.; Hansen, E.; Andersen, J.H.; Kristiansen, P.E.; Haug, T., J. Nat. Prod. 2011, 74, 837-841.
3). Rahbaek, L.; Anthoni, U.; Christophersen, G.; Nielsen, P.H.; Petersen, B.O., J Org. Chem. 1996, 61, 887-889.
4). Rahbæk, L.; Christophersen, C, . J. Nat. Prod. 1997, 60, 175-177.

UNIVERSITY OF TROMSØ